

**Probabilities in Quantum Cosmological Models:
A Decoherent Histories Analysis Using a Complex Potential**

J.J.Halliwel

Blackett Laboratory

Imperial College

London SW7 2BZ

UK

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Abstract

In the quantization of simple cosmological models (minisuperspace models) described by the Wheeler-DeWitt equation, an important step is the construction, from the wave function, of a probability distribution answering various questions of physical interest, such as the probability of the system entering a given region of configuration space at any stage in its entire history. A standard but heuristic procedure is to use the flux of (components of) the wave function in a WKB approximation. This gives sensible semiclassical results but lacks an underlying operator formalism. In this paper, we address the issue of constructing probability distributions linked to the Wheeler-DeWitt equation using the decoherent histories approach to quantum theory. The key step is the construction of class operators characterizing questions of physical interest. Taking advantage of a recent decoherent histories analysis of the arrival time problem in non-relativistic quantum mechanics, we show that the appropriate class operators in quantum cosmology are readily constructed using a complex potential. The class operator for not entering a region of configuration space is given by the S -matrix for scattering off a complex potential localized in that region. We thus derive the class operators for entering one or more regions in configuration space. The class operators commute with the Hamiltonian, have a sensible classical limit and are closely related to an intersection number operator. The definitions of class operators given here handles the key case in which the underlying classical system has multiple crossings of the boundaries of the regions of interest. We show that oscillatory WKB solutions to the Wheeler-DeWitt equation give approximate decoherence of histories, as do superpositions of WKB solutions, as long as the regions of configuration space are sufficiently large. The corresponding probabilities coincide, in a semiclassical approximation, with standard heuristic procedures. In brief, we exhibit the well-defined operator formalism underlying the usual heuristic interpretational methods in quantum cosmology.

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I. INTRODUCTION

A. Opening Remarks

A question in quantum gravity that continues to attract considerable interest is the problem of quantizing and interpreting the Wheeler-DeWitt equation of minisuperspace quantum cosmology [1–5],

$$H\Psi = 0 \tag{1.1}$$

Although the setting of this problem is simple cosmological models with just a handful of homogeneous parameters, the techniques employed in answering this question may be relevant to general approaches to quantum gravity, such as the loop variables approach or causal set approach. This is because the central difficulty in consistently quantizing and interpreting the Wheeler-DeWitt equation is the absence of a variable to play the role of time and all approaches to quantum gravity must confront this issue at some stage [6].

A frequently studied example consists of a closed FRW cosmology with scale factor $a = e^\alpha$ and a homogeneous scalar field ϕ with (inflationary) potential $V(\phi)$ [7]. The Wheeler-DeWitt equation for this model is

$$\left(\frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} + e^{6\alpha} V(\phi) - e^{4\alpha} \right) \Psi(\alpha, \phi) = 0 \tag{1.2}$$

Given suitable boundary conditions, one can solve this equation for the wave function $\Psi(\alpha, \phi)$ and attempt to use it to answer a number of interesting cosmological questions. There are many such questions: Is there a regime in which the universe behaves approximately classically? What is the probability that the universe expands beyond a given size a_0 ? What is the probability that the universe has a certain energy density at a given value of the scale factor? What is the probability that the universe’s history passes through a given region Δ of configuration space, characterized by certain ranges of a and ϕ ?

Such questions, of necessity, do not involve the specification of an external time. Classically, the system’s trajectories in minisuperspace may be written as paths $(\alpha(t), \phi(t))$, but here t is a convenient but unphysical parameter that labels the points along the paths – it does not correspond to the physical time measured by an external clock. The absence of a physical time is reflected in the quantum theory by the fact that the quantum state obeys the Wheeler-DeWitt equation Eq.(1.1), not a Schrödinger equation, and it is this difference that presents such a challenge to conventional quantization methods.

Although very plausible heuristic semiclassical methods exist for formulating and answering the above questions (in particular, the WKB interpretation [1]), it is of interest to see whether or not there exists a precise and well-defined quantum-mechanical scheme underlying these heuristic methods. We are not looking for high standards of mathematical rigour – just a standard quantum-mechanical framework of operators, inner product structures etc, obeying some reasonable requirements. The purpose of this paper is to show, building on earlier attempts [8–15], that such a framework exists in the context of the decoherent histories approach to quantum theory.

B. Inner Products and Operators for the Wheeler-DeWitt Equation

In the Wheeler-DeWitt equation (1.1), H is the Hamiltonian operator of a minisuperspace model with n coordinates q^a , and is typically of the form

$$H = -\nabla^2 + U(q) \quad (1.3)$$

where ∇ is the Laplacian in the minisuperspace metric f_{ab} , which has signature $(-+++ \dots)$. It is naturally linked to the current,

$$J_a = i \left(\Psi^* \overrightarrow{\partial}_a \Psi - \Psi^* \overleftarrow{\partial}_a \Psi \right) \quad (1.4)$$

which is conserved

$$\nabla \cdot J = 0 \quad (1.5)$$

Closely associated is the Klein-Gordon inner product defined on a surface Σ

$$(\Psi, \Phi)_{KG} = i \int_{\Sigma} d\sigma^a \left(\Psi^* \overrightarrow{\partial}_a \Phi - \Psi^* \overleftarrow{\partial}_a \Phi \right) \quad (1.6)$$

where $d\sigma^a$ is a surface element normal to Σ . In flat space with a constant potential, the Wheeler-DeWitt equation is just the Klein-Gordon equation. Its solutions may be sorted out into positive and negative frequency in the usual way. With a little attention to sign, it is then possible to use components of the current to define probabilities.

However, in general, it is not possible to sort the solutions to the Wheeler-DeWitt equation into positive and negative frequency. This is one manifestation of the problem of time and more elaborate methods are required to associate probabilities with the Wheeler-DeWitt

equation. There are two main issues: finding an inner product, and then finding suitable operators.

The issue of finding a suitable positive inner product is reasonably straightforward and goes by the name of Rieffel induction, or the induced (or physical) inner product [9, 16]. We consider first the usual Schrödinger inner product,

$$\langle \Psi_1 | \Psi_2 \rangle = \int d^n q \Psi_1^*(q) \Psi_2(q) \quad (1.7)$$

We then consider eigenvalues of the Wheeler-DeWitt operator

$$H|\Psi_{\lambda k}\rangle = \lambda|\Psi_{\lambda k}\rangle \quad (1.8)$$

where k labels the degeneracy. These eigenstates will satisfy

$$\langle \Psi_{\lambda' k'} | \Psi_{\lambda k} \rangle = \delta(\lambda - \lambda') \delta(k - k') \quad (1.9)$$

from which it is clear that this inner product diverges when $\lambda = \lambda'$. The induced inner product on a set of eigenstates of fixed λ is defined, loosely speaking, by discarding the δ -function $\delta(\lambda - \lambda')$. That is, the induced (or physical) inner product is then defined by

$$\langle \Psi_{\lambda k'} | \Psi_{\lambda k} \rangle_{phys} = \delta(k - k') \quad (1.10)$$

This procedure can be defined quite rigorously, and has been discussed at some length in Refs.[9, 16]. It is readily shown that the induced inner product coincides with the Klein-Gordon inner product when a division into positive and negative frequencies is possible, with the signs adjusted to make it positive. (This is described in Appendix A).

Turning now to the construction of interesting operators, the interesting dynamical variables associated with the Wheeler-DeWitt equation are those that commute with H . This is because the constraint equation is related to reparametrization invariance – which is reflected in the absence of a physical time variable – and we seek operators which are invariant. A wide class of operators commuting with H are of the form

$$A = \int_{-\infty}^{\infty} dt B(t) \quad (1.11)$$

which clearly commute with H since

$$\begin{aligned} e^{iHs} A e^{-iHs} &= \int_{-\infty}^{\infty} dt B(t+s) \\ &= A \end{aligned} \quad (1.12)$$

Many examples are given in Refs.[5, 11, 16]. However, another way of constructing such operators involves taking products,

$$A = \prod_{t=-\infty}^{\infty} B(t) \quad (1.13)$$

which may be shown to commute with H using essentially the same argument [12], but clearly further mathematical detail is required to give meaning to the infinite product. (Here t is the unphysical parameter time).

Given these prescriptions for inner products and operators, one may then attempt to construct operators and probabilities implementing some of the questions mentioned above. We will focus on the following general question: Given a solution Ψ to the Wheeler-DeWitt equation, what is the probability of finding the system in a region Δ of configuration space, or of crossing a surface Σ , at any stage in the system's history? The question is depicted in Figure 1.

Questions involving surface crossings are not unlike more familiar questions in non-relativistic quantum mechanics, where there is a physical time parameter, but the key difference in quantum cosmology is that even classically, a given trajectory will typically cross a fixed surface more than once. It is precisely these sorts of issues that need to be carefully phrased in the quantum theory. Whilst the operator formalism briefly outlined above has been used to address such questions [5], the problems of characterizing properties of trajectories and surface crossings in quantum theory is naturally accommodated in the decoherent histories approach to quantum theory.

C. The Decoherent Histories Approach

A more general approach to quantizing and interpreting the Wheeler-DeWitt equation is provided by the decoherent histories approach to quantum theory, and this approach will be the focus of this paper [17–25]. In this approach, probabilities are assigned to histories using the formula

$$p(\alpha) = \text{Tr} (C_\alpha \rho C_\alpha^\dagger) \quad (1.14)$$

Here, ρ is the initial state (in our case a pure state) and C_α is a class operator characterizing the histories α of interest. In non-relativistic quantum mechanics these class operators are

given by time-ordered strings of projection operators,

$$C_\alpha = P_{\alpha_n}(t_n) \cdots P_{\alpha_2}(t_2) P_{\alpha_1}(t_1) \quad (1.15)$$

(or by sums of such strings). The class operators always satisfy the condition

$$\sum_{\alpha} C_\alpha = 1 \quad (1.16)$$

For the reparameterization invariant systems considered here, the definition of the class operators is more subtle, and we return to this below.

Because of interference between pairs of histories, probabilities cannot always be assigned. To check for interference we therefore consider the decoherence functional,

$$D(\alpha, \alpha') = \text{Tr} \left(C_\alpha \rho C_{\alpha'}^\dagger \right) \quad (1.17)$$

When

$$D(\alpha, \alpha') = 0 \quad (1.18)$$

for all pairs of histories in the set with $\alpha \neq \alpha'$, we say that there is decoherence of the set of histories and probabilities may be assigned Eq.(1.14). When there is decoherence, it is easily seen from Eq.(1.16) that the probabilities Eq.(1.14) are also given by

$$p(\alpha) = \text{Tr} (C_\alpha \rho) = \text{Tr} (C_\alpha^\dagger \rho) \quad (1.19)$$

Decoherence guarantees that this expression is real and positive, even though the class operators are not positive or hermitian operators in general.

The structure of the decoherent histories approach is very general and may be applied to a wide variety of situations, given an initial state, class operators, and a suitable inner product structure. For the application to the Wheeler-DeWitt system considered here, the initial state is taken to be a solution to the Wheeler-DeWitt equation and the inner product is the induced inner product described above.

The most crucial element is the specification of the class operators C_α . In non-relativistic quantum theory, the class operator is generally a string of projection operators like Eq.(1.15), or a sum of strings of such operators, but this basic structure can be generalized in various ways. The product in the string can be taken to be continuous time [25]. Also, it is often valuable, sometimes essential, to allow the projectors to be replaced by more general

operators, such as POVMs. The class operators must also properly characterize the histories one is interested in. It is not always obvious how to do this but useful clues often come from looking at the classical analogue of the class operator (where all the projectors commute).

Here, we are interested in histories which enter a region Δ of configuration space, or which cross a surface Σ , but without regard to time. This absence of a physical time variable seems particularly challenging, given that time seems to be central to the definition of non-relativistic analogue, Eq.(1.15). Closely related to this is the role of the constraint equation, Eq.(1.1). As noted already, these two features are directly related to the underlying symmetry of the theory – reparametrization invariance – and this symmetry is respected if the class operators commute with the constraint,

$$[H, C_\alpha] = 0 \tag{1.20}$$

Eq.(1.20) is in keeping with standard procedures of Dirac quantization [5]) and also ensures that the class operators have a sensible classical limit [12].

Some partially successful attempts to construct such class operators have been given previously [9–12], but ran into various problems to do with the Zeno effect and with compatibility with the constraint equation. The main aim of this paper is to give fully satisfactory definitions of class operators for quantum cosmological models and explore their decoherence properties and probabilities.

D. Some Properties of the Wheeler-DeWitt Equation and the WKB Interpretation

To prepare the way for the full decoherent histories analysis of quantum cosmology, it is important to discuss some properties of the Wheeler-DeWitt equation and review the commonly used heuristic semiclassical interpretation of the wave function, since a proper quantization must recover this structure in some limit.

The Wheeler-DeWitt equation Eq.(1.3) is a Klein-Gordon equation in a curved configuration space with indefinite metric $f_{ab}(q)$ and potential $U(q)$ which can be positive or negative. The curvature effects of the metric are not significant in relation to the issues addressed in this paper, so we will assume for simplicity that the metric is flat.

The classical constraint equation corresponding to the Wheeler-DeWitt equation Eq.(1.3)

is

$$\frac{1}{4}f_{ab}\dot{q}^a\dot{q}^b + U = 0 \quad (1.21)$$

from which one can see that the classical trajectories are timelike in the region $U > 0$ and spacelike in $U < 0$. (The timelike direction is that of increasing scale factor and the spacelike directions correspond to matter and anisotropic modes). The quantum case has analogous features. In simple models such as Eq.(1.2), the character of the solutions to the Wheeler-DeWitt equation depends on the sign of U . For large scale factors, $U > 0$ and the wave function is oscillatory, corresponding, very loosely, to a quasiclassical regime, and for small scale factors, $U < 0$, and the wave function is exponential, corresponding to a classical forbidden regime. However, there are certain types of models (such as those with an exponential potential for the scalar field), in which the identification of the oscillatory and exponential regions depends also on whether the constant U surfaces are spacelike or timelike [26]. We will not address this here.

One can also associate a Feynman propagator G_F with the Wheeler-DeWitt operator,

$$\begin{aligned} G_F &= \int_0^\infty dt e^{-iHt - \epsilon t} \\ &= \frac{-i}{H - i\epsilon} \end{aligned} \quad (1.22)$$

where $\epsilon \rightarrow 0+$. (Numerous propagator-like objects of this type have been considered in quantum cosmology [27]). Locally, on scales smaller than the scale on which the potential U significantly varies, the propagator $G_F(q, q')$ will be essentially identical in its properties with the analogous object for the relativistic particle for flat space. Therefore, in the region $U > 0$, for points q and q' which are timelike separated, it will propagate positive frequency solutions to the future and negative frequency solutions to the past. It will be exponentially suppressed for initial and final points q and q' which are spacelike separated (this is the familiar “propagation outside the lightcone” effect). For $U < 0$, similar statements hold but with timelike and spacelike reversed. Similar features hold on larger scales in a semiclassical approximation. These properties are important to understand the class operator constructed below.

Very plausible but heuristic answers to questions concerning crossing surfaces and entering regions are readily found using the WKB approximate solutions to the Wheeler-DeWitt equation and the Klein-Gordon current [1]. In the oscillatory regime, the Wheeler-DeWitt

equation may be solved using the WKB ansatz

$$\Psi = R e^{iS} \quad (1.23)$$

where the rapidly varying phase S obeys the Hamilton-Jacobi equation

$$(\nabla S)^2 + U = 0 \quad (1.24)$$

and the slowly varying prefactor R obeys

$$\nabla \cdot (|R|^2 \nabla S) = 0 \quad (1.25)$$

The latter equation is just current conservation for the WKB current,

$$J = |R|^2 \nabla S \quad (1.26)$$

Wave functions of the WKB form Eq.(1.23) indicate a correlation between position and momenta of the form

$$p = \nabla S \quad (1.27)$$

and this suggests that the wave function Eq.(1.23) corresponds to an ensemble of classical trajectories satisfying Eq.(1.27). The current J may then be used to define a measure on this set of trajectories. For example, we consider a surface Σ and choose the normal n^a to the surface so that $n \cdot \nabla S > 0$. Then the probability of the system crossing the surface is taken to be

$$p(\Sigma) = \int_{\Sigma} d^{n-1}q \, n^a J_a \quad (1.28)$$

Of particular interest here is the probability of entering a region Δ . This is clearly related to the flux at the boundary of the region. The current will typically intersect the boundary of Δ *twice*. However, we can split the boundary Σ of Δ into two sections: Σ_{in} at which the current is ingoing and Σ_{out} at which the current is outgoing. The probability of entering Δ is may then be expressed in the two forms

$$\begin{aligned} p(\Delta) &= - \int_{\Sigma_{in}} d^{n-1}q \, n^a J_a \\ &= \int_{\Sigma_{out}} d^{n-1}q \, n^a J_a \end{aligned} \quad (1.29)$$

where here we have defined the normal n^a to point outwards. See Figure 2. These two forms are equivalent since the current is locally conserved.

Typically, little is said of the regions in which the wave function is exponential, except that they are similar to tunneling regions in non-relativistic quantum mechanics, so are classically forbidden in some sense. However, the wave function is not necessarily small in these regions, so there is surely more to it than this. In Ref.[28], it was noted that, unlike the oscillatory regions, the exponential regions do not indicate a correlation between position and momenta of the form Eq.(1.27), and it seems that this should be significant in some way.

Whilst the WKB interpretation is very plausible and adequate for most situations of interest, it leaves many questions unanswered. The main issue is to understand the operator origin of these probabilities, in terms of the language of operators commuting with H developed above. Furthermore, what can one say about superpositions of WKB states? Can interference between them be neglected? Also, what can one say about the exponential, classically forbidden regions? Is there a more precise way of saying that they are non-classical?

E. This Paper

The purpose of this paper is to present a decoherent histories quantization of the Wheeler-DeWitt equation, and in particular to exhibit exactly defined class operators which characterize histories entering regions of configuration space or crossing surfaces, without reference to an external time. The key idea is to use a complex potential to define the class operator for not entering a region Δ in configuration space. In particular, we take the class operator for not entering to be the S matrix describing scattering off a complex potential localized in Δ . This turns out to have all the right properties and to give physically sensible results for decoherence and probabilities.

In Section 2, to explain and motivate the use of a complex potential we review the use of such potentials in the decoherent histories analysis of the arrival time problem in non-relativistic quantum mechanics. In Section 3, we describe the construction of class operators for the Wheeler-DeWitt equation using a complex potential. The properties of the class operator for entering a region Δ are described in Section 4. The class operator has a sensible classical limit which, crucially, registers just one intersection of a trajectory with a surface, even when the trajectory intersects twice or more. In the quantum case, the

class operator is an operator describing the ingoing flux across the boundary of the region, an expected result on semiclassical grounds, and is closely related to an intersection number operator.

In Section 5, some simple one and two dimensional examples are considered in detail to confirm the properties of the class operator outlined in Section 4. We also confirm that the formalism gives sensible and expected results for surface crossings of the relativistic particle in flat space. In Section 6 we consider the WKB regime and show that the decoherent histories analysis reproduces the expected heuristic interpretation of the wave function. We summarize and conclude in Section 7. Some properties of the inner product structure of the Klein-Gordon equation are summarized in Appendix A.

II. THE ARRIVAL TIME PROBLEM IN NON-RELATIVISTIC QUANTUM THEORY

In this section we summarize some of the key features of the arrival time problem in non-relativistic quantum mechanics [29]. These details are very relevant to the quantum cosmology case and in particular motivate the use of complex potentials in the definition of class operators.

In the one-dimensional statement of the arrival time problem, one considers an initial wave function $|\psi\rangle$ concentrated in the region $x > 0$ and consisting entirely of negative momenta. The question is then to find the probability $\Pi(\tau)d\tau$ that the particle crosses $x = 0$ between time τ and $\tau + d\tau$. See Figure 3. The canonical answer is the current density

$$J(\tau) = \frac{(-1)}{2m} \langle \psi_\tau | (\hat{p}\delta(\hat{x}) + \delta(\hat{x})\hat{p}) | \psi_\tau \rangle \quad (2.1)$$

where $|\psi_\tau\rangle$ is the freely evolved state. This has the correct semiclassical limit, but can be negative for certain types of states consisting of superpositions of different momenta (back-flow states). It is of interest to explore whether this simple semiclassical result emerges from more elaborate measurement-based or axiomatic schemes. Many such schemes naturally lead to the use of a complex potential $-iV(x)$ in the Schrödinger equation [30], where

$$V(x) = V_0\theta(-x) \quad (2.2)$$

With such a potential, the state at time τ is

$$|\psi(\tau)\rangle = \exp(-iH\tau - V_0\theta(-x)\tau) |\psi\rangle \quad (2.3)$$

where H is the free Hamiltonian. The idea here is that the part of the wave packet that reaches the origin during the time interval $[0, \tau]$ should be absorbed, so that $\langle \psi(\tau) | \psi(\tau) \rangle$ is the probability of not crossing $x = 0$ during the time interval $[0, \tau]$. The probability of crossing between τ and $\tau + d\tau$ is then

$$\Pi(\tau) = -\frac{d}{d\tau} \langle \psi(\tau) | \psi(\tau) \rangle \quad (2.4)$$

This may be approximately evaluated in the limit $V_0 \ll E$ (where E is the typical energy scale), which is the limit of negligible reflection off the complex potential. The result is

$$\Pi(\tau) = 2V_0 \int_0^\tau dt e^{-2V_0(\tau-t)} J(t) \quad (2.5)$$

The probability for crossing during a finite interval $[\tau_1, \tau_2]$ is then given by

$$p(\tau_2, \tau_1) = \int_{\tau_1}^{\tau_2} d\tau \Pi(\tau) \quad (2.6)$$

and if this time interval is sufficiently large compared to $1/V_0$, we have

$$p(\tau_2, \tau_1) \approx \int_{\tau_1}^{\tau_2} dt J(t) \quad (2.7)$$

which means that the dependence on the potential drops out entirely at sufficiently coarse grained scales, and there is agreement with semiclassical expectations involving the current $J(t)$.

In the decoherent histories analysis of the arrival time problem [31, 32], we first consider the construction of the class operator C_{nc} for not crossing the origin during the finite time interval $[0, \tau]$. We split the time interval into N parts of size ϵ , and the class operator is provisionally defined by

$$C_{nc} = P e^{-iH\epsilon} P \dots e^{-iH\epsilon} P \quad (2.8)$$

where there are $N+1$ projections $P = \theta(\hat{x})$ onto the positive x -axis and N unitary evolution operators in between. One might be tempted to take the limit $N \rightarrow \infty$ and $\epsilon \rightarrow 0$, but this yields physically unreasonable results. This limit actually yields the restricted propagator in $x > 0$,

$$\begin{aligned} C_{nc} &= g_r(\tau, 0) \\ &= P e^{-iPHP\tau} \end{aligned} \quad (2.9)$$

This object is also given by the path integral expression

$$\langle x_1 | g_r(\tau, 0) | x_0 \rangle = \int_r \mathcal{D}x \exp(iS) \quad (2.10)$$

where the integral is over all paths from $x(0) = x_0$ to $x(\tau) = x_1$ that always remain in $x(t) > 0$. However, the class operator defined by Eq.(2.9) has a problem with the Zeno effect – it consists of continual projections onto the region $x > 0$ and as a result the wave function never leaves the region. This is reflected in the fact that the restricted propagator g_r is unitary in the Hilbert space of states with support only in $x > 0$. This is a serious difficulty which has plagued a number of earlier works in this area [33–35].

To avoid the Zeno effect, the key is to keep ϵ finite, and in particular, standard wisdom suggests that $\epsilon > 1/\Delta H$, where H is the free particle Hamiltonian. The class operator Eq.(2.8) is not easy to work with for finite ϵ , but fortunately an extremely useful result of Echanobe et al. comes to the rescue [36]. They argued that the string of operators in Eq.(2.8) is in fact approximately equivalent to evolution in the presence of the complex potential $-iV$ introduced above. That is,

$$P e^{-iH\epsilon} P \dots e^{-iH\epsilon} P \approx \exp(-iH_0\tau - V_0\theta(-\hat{x})\tau) \quad (2.11)$$

They argued that this is valid for $\Delta H \ll V_0$ and $V_0\epsilon \gg 1$, but there is evidence that this connection is valid more generally [37]. In any event it strongly suggests that the class operator C_{nc} , normally defined by a string of projection operators, is justifiably defined instead using a complex potential. That is, we define

$$C_{nc} = \exp(-iH_0\tau - V_0\theta(-\hat{x})\tau) \quad (2.12)$$

The subsequent decoherent histories analysis was described in detail in Ref.[31]. The corresponding class operator for crossing during a time interval $[\tau_1, \tau_2]$ was shown to be

$$C_c(\tau_2, \tau_1) = \int_{\tau_1}^{\tau_2} dt e^{-iH_0(\tau-t)} V e^{-iH_0t-Vt} \quad (2.13)$$

and again in the approximation $V_0 \ll E$ and for time intervals greater than $1/V_0$ this may be shown to have the simple and appealing form

$$C_c(\tau_2, \tau_1) \approx \int_{\tau_1}^{\tau_2} dt e^{-iH\tau} \frac{(-1)}{2m} (\hat{p} \delta(\hat{x}_t) + \delta(\hat{x}_t) \hat{p}) \quad (2.14)$$

which is now independent of the V_0 . (These definitions of class operators differ by a factor of $\exp(-iH\tau)$ from those defined in Section 1C, but this does not make any difference in the

decoherence functional and probabilities). With this class operator, one can show that there is decoherence of histories for a variety of interesting initial states, such as wave packets (but not for superposition states with backflow), and for such states, the general result Eq.(1.19) implies that the probability for crossing is simply

$$p(\tau_2, \tau_1) = \langle \Psi | C_c(\tau_2, \tau_1) | \Psi \rangle \quad (2.15)$$

which agrees precisely with the semiclassical expected result, Eq.(2.7).

In summary, the decoherent histories analysis of the arrival time problem in non-relativistic quantum mechanics indicates that it is reasonable to define class operators for not entering a space time region using a complex potential, as in Eq.(2.12), and that such a definition gives sensible a semiclassical limit, independent of the potential, at sufficiently coarse grained scales.

III. CONSTRUCTION OF THE CLASS OPERATORS USING A COMPLEX POTENTIAL

We now come to the central issue concerning this paper, which is the construction of class operators for the decoherent histories analysis of the Wheeler-DeWitt equation.

A. Class Operators for a Single Region

We seek class operators for the system Eq.(1.3) describing histories which enter or do not enter the region Δ , without specification of the time at which they enter. It is easiest to first focus on the class operator \bar{C}_Δ for not entering and the class operator for entering is then given by

$$C_\Delta = 1 - \bar{C}_\Delta \quad (3.1)$$

The earliest attempts to define class operators for the Wheeler-DeWitt equation involved defining \bar{C}_Δ as a sort of propagator obtained by integrating restricted propagators of the form Eq.(2.10) over an infinite range t (now regarded as the unphysical parameter time) [9–11]. However, in addition to having problems with the Zeno effect (which was not in fact appreciated in these earlier works), such constructions are difficult to reconcile with the

constraint equation and some ad hoc modifications of the basic construction were required to give sensible answers.

A rather different approach to constructing \bar{C}_Δ was given in Ref.[12]. This was again problematic, but we review the construction here, since it is readily modified to yield a successful definition of the class operators. We denote by P the projector onto Δ and \bar{P} the projector onto the outside of Δ . Our provisional proposal for the class operator for trajectories not entering Δ is the time-ordered infinite product,

$$\bar{C}_\Delta = \prod_{t=-\infty}^{\infty} \bar{P}(t) \quad (3.2)$$

where t is the unphysical parameter time. Subject to a more precise definition, given shortly, this object has the required properties. It is a string of projectors. Classically, it is equal to one for trajectories which remain outside Δ at every moment of parameter time. Also, it commutes with H , at least formally.

To define this more precisely, we first consider the product of projectors at a discrete set of times, $t_1, t_1 + \epsilon, t_1 + 2\epsilon, \dots, t_1 + n\epsilon = t_2$. We define the intermediate quantity, $\bar{C}_\Delta(t_2, t_1)$ as the continuum limit of the product of projectors,

$$\bar{C}_\Delta(t_2, t_1) = \lim_{\epsilon \rightarrow 0} \bar{P}(t_2) \bar{P}(t_2 - \epsilon) \dots \bar{P}(t_1 + \epsilon) \bar{P}(t_1) \quad (3.3)$$

where the limit is $n \rightarrow \infty, \epsilon \rightarrow 0$ with $t_2 - t_1$ fixed. The desired class operator is then

$$\bar{C}_\Delta = \lim_{t_2 \rightarrow \infty, t_1 \rightarrow -\infty} \bar{C}_\Delta(t_2, t_1) \quad (3.4)$$

The class operator operator is clearly closely related to the restricted propagator g_r (the generalization of Eq.(2.10)) in the region outside Δ , since we have

$$\bar{C}_\Delta(t_2, t_1) = e^{iHt_2} g_r(t_2, t_1) e^{-iHt_1} \quad (3.5)$$

and therefore

$$\bar{C}_\Delta = \lim_{t_2 \rightarrow \infty, t_1 \rightarrow -\infty} e^{iHt_2} g_r(t_2, t_1) e^{-iHt_1} \quad (3.6)$$

The class operator commutes with H . This is because, from Eq.(3.5)

$$e^{iHs} \bar{C}_\Delta(t_2, t_1) e^{-iHs} = e^{iH(t_2+s)} g_r(t_2, t_1) e^{-iH(t_1+s)} \quad (3.7)$$

This becomes independent of s as $t_2 \rightarrow \infty, t_1 \rightarrow -\infty$, hence

$$[H, \bar{C}_\Delta] = 0 \quad (3.8)$$

The problem with this definition, however, is that it suffers from the Zeno effect, exactly like the analogous expression Eq.(2.8) (in the limit $\epsilon \rightarrow 0$) in the non-relativistic arrival time problem. But the key idea here is that we may also get around the problem in the same way, using a complex potential. That is, we “soften” the restricted propagator and make the replacement

$$g_r(t_2, t_1) \rightarrow \exp(-iH(t_2 - t_1) - V(t_2 - t_1)) \quad (3.9)$$

where $V(q) = V_0 f_\Delta(q)$. Here, $V_0 > 0$ is a constant and $f_\Delta(q)$ is the characteristic function of Δ , so is 1 in Δ and 0 outside it. Or we may equivalently write $V = V_0 P$, where recall, P is the projector onto Δ . This means that our new definition for the class operator is

$$\bar{C}_\Delta = \lim_{t_2 \rightarrow \infty, t_1 \rightarrow -\infty} e^{iHt_2} \exp(-i(H - iV)(t_2 - t_1)) e^{-iHt_1} \quad (3.10)$$

The class operator thus defined has an appealing form: it is the S-matrix for system with Hamiltonian Eq.(1.3) scattering off the complex potential V . As required, it commutes with H . This is the most important definition of the paper.

Now an important observation. The class operator derived above has been defined as a time-ordered product of operators in which the direction of parameter time increases from right to left. However, since parameter time is unphysical, there is absolutely no reason why the parametrization should not run in the opposite direction. This produces an operator which is the hermitian conjugate of Eq.(3.10). As one can see from Eq.(1.19), this makes no difference in the final expressions for probabilities. In fact, it is most natural to define the class operator in such a way that it is invariant under reversing the direction of parametrization. We thus define a modified class operator which is hermitian:

$$\bar{C}'_\Delta = \frac{1}{2} (\bar{C}_\Delta + \bar{C}_\Delta^\dagger) \quad (3.11)$$

In what follows, for simplicity, we will primarily work with the non-hermitian class operator Eq.(3.10) and revert to the hermitian one, Eq.(3.11) where appropriate. The difference between them will turn out to be significant only for the class operator for two or more regions.

We now cast the above class operator in a more useable form. The following identities

are readily derived:

$$e^{-i(H-iV)(t_2-t_1)} = e^{-iH(t_2-t_1)} - \int_{t_1}^{t_2} dt e^{-iH(t_2-t)} V e^{-i(H-iV)(t-t_1)} \quad (3.12)$$

$$= e^{-iH(t_2-t_1)} - \int_{t_1}^{t_2} dt e^{-i(H-iV)(t_2-t)} V e^{-iH(t-t_1)} \quad (3.13)$$

Inserting the second expression in the first, we obtain

$$\begin{aligned} e^{-i(H-iV)(t_2-t_1)} &= e^{-iH(t_2-t_1)} - \int_{t_1}^{t_2} dt e^{-iH(t_2-t)} V e^{-iH(t-t_1)} \\ &\quad + \int_{t_1}^{t_2} dt \int_{t_1}^t ds e^{-iH(t_2-t)} V e^{-i(H-iV)(t-s)} V e^{-iH(s-t_1)} \end{aligned} \quad (3.14)$$

Inserting in the expression for the class operator (3.10) and taking the limit, we obtain

$$\begin{aligned} \bar{C}_\Delta &= 1 - \int_{-\infty}^{\infty} dt V(t) \\ &\quad + \int_{-\infty}^{\infty} dt \int_{-\infty}^t ds e^{iHt} V e^{-i(H-iV)(t-s)} V e^{-iHs} \end{aligned} \quad (3.15)$$

The class operator for entering the region is therefore given by

$$C_\Delta = \int_{-\infty}^{\infty} dt V(t) - \int_{-\infty}^{\infty} dt \int_{-\infty}^t ds e^{iHt} V e^{-i(H-iV)(t-s)} V e^{-iHs} \quad (3.16)$$

This is an exact and useful form for the class operator for entering Δ , and it is easily confirmed that it is of the form Eq.(1.11) so commutes with H .

Now we use a simple but useful semiclassical approximation. Noting that $V = V_0 P$, where P recall projects into Δ , note that the expression

$$V e^{-i(H-iV)(t-s)} V \quad (3.17)$$

describes propagation with the complex Hamiltonian $H - iV$ between two points that lie inside Δ . This can easily be represented by a path integral in which it seems plausible that the dominant paths between this two end-points will lie entirely inside Δ , as long as the boundary is reasonable smooth and the semiclassical paths are not too irregular. If this is true, we may replace $V = V_0 P$ by the constant complex potential $V = V_0$, that is,

$$V e^{-i(H-iV)(t-s)} V \approx V e^{-i(H-iV_0)(t-s)} V \quad (3.18)$$

Propagation with a complex potential in Eq.(3.17) will also involve reflection off the boundary of the region, in which case the semiclassical approximation Eq.(3.18) may fail. However,

reflection is small for sufficiently small V_0 [30, 31], and we will see this in more detail in Section 5. Hence we expect the semiclassical approximation Eq.(3.18) to hold for small V_0 .

With this useful approximation (which does not affect the fact that the class operator commutes with H), we have

$$C_\Delta = \int_{-\infty}^{\infty} dt V(t) - \int_{-\infty}^{\infty} dt \int_{-\infty}^t ds V(t)V(s)e^{-V_0(t-s)} \quad (3.19)$$

Again using $V = V_0 P$, this is easily rewritten

$$C_\Delta = \int_{-\infty}^{\infty} dt P(t) \int_{-\infty}^t ds V_0 e^{-V_0(t-s)} \dot{P}(s) \quad (3.20)$$

This is the main result of the paper: a class operator commuting with H , describing histories which enter the region Δ . It is valid in the approximation Eq.(3.18), which is sufficient to cover the key case of histories which, classically, intersect the boundary of Δ twice.

For systems whose classical paths intersect the surfaces of interest more than two times, the semiclassical approximation Eq.(3.18) will not be valid, but the exact result Eq.(3.16) may still be used. It may also be of interest to explore higher order semiclassical approximations obtained by iterations of the basic result Eq.(3.14). This will not be explored here.

B. Class Operators for Two Regions

We now extend the above results to the case of histories which enter two regions, Δ_1, Δ_2 where we define P_1 and P_2 to be the projection operators onto these regions. We proceed as follows. The class operator Eq.(3.15) is defined for any complex potential V so we may use a potential

$$\begin{aligned} V &= V_1 + V_2 \\ &= V_{10}P_1 + V_{20}P_2 \end{aligned} \quad (3.21)$$

which has support only in the regions Δ_1, Δ_2 . Here V_{10} and V_{20} are positive constants. This potential inserted in Eq.(3.15) defines the class operator $\bar{C}_{\Delta_1\Delta_2}$ for histories which remain outside of both Δ_1 and Δ_2 . The negation of this class operator therefore describes histories which enter Δ_1 or Δ_2 , or both, and we may write

$$\bar{C}_{\Delta_1\Delta_2} = 1 - C_{\Delta_1} - C_{\Delta_2} - C_{\Delta_1\Delta_2} \quad (3.22)$$

Here, C_{Δ_1} and C_{Δ_2} are the class operators for entering the regions Δ_1 , Δ_2 and are given by expressions of the form Eq.(3.16). We may thus deduce the form of the class operator $C_{\Delta_1\Delta_2}$ for entering both regions.

The class operator Eq.(3.15) with the potential Eq.(3.21) is

$$\begin{aligned}\bar{C}_{\Delta_1\Delta_2} = & 1 - \int_{-\infty}^{\infty} dt (V_1(t) + V_2(t)) \\ & + \int_{-\infty}^{\infty} dt \int_{-\infty}^t ds e^{iHt}(V_1 + V_2)e^{-i(H-i(V_1+V_2))(t-s)}(V_1 + V_2)e^{-iHs}\end{aligned}\quad (3.23)$$

It seems reasonable to make the semiclassical approximations

$$V_1 e^{-i(H-i(V_1+V_2))(t-s)} V_1 \approx V_1 e^{-i(H-iV_1)(t-s)} V_1 \quad (3.24)$$

$$V_2 e^{-i(H-i(V_1+V_2))(t-s)} V_2 \approx V_2 e^{-i(H-iV_2)(t-s)} V_2 \quad (3.25)$$

These approximations are very similar to Eq.(3.18). Eq.(3.24) is essentially the notion that the propagator between two points in Δ_1 will involve negligible contribution from paths that enter Δ_2 . Similarly for Eq.(3.25). With these approximations we can easily identify the terms C_{Δ_1} and C_{Δ_2} and we deduce

$$\begin{aligned}C_{\Delta_1\Delta_2} = & - \int_{-\infty}^{\infty} dt \int_{-\infty}^t ds e^{iHt} V_2 e^{-i(H-i(V_1+V_2))(t-s)} V_1 e^{-iHs} \\ & - \int_{-\infty}^{\infty} dt \int_{-\infty}^t ds e^{iHt} V_1 e^{-i(H-i(V_1+V_2))(t-s)} V_2 e^{-iHs}\end{aligned}\quad (3.26)$$

To estimate the propagator

$$V_2 e^{-i(H-i(V_1+V_2))(t-s)} V_1 \quad (3.27)$$

we need a semiclassical approximation more elaborate than Eq.(3.18), since it involves propagation from an initial point in Δ_1 with potential V_1 , to a final point in Δ_2 with potential V_2 but with zero complex potential outside these regions. The path decomposition expansion [38–40] is naturally adapted to this problem, since it is a tool for breaking up a propagator into its properties in different spatial regions. We will simply write down the result of using this expansion, with some brief justification.

$$\begin{aligned}P_2 e^{-i(H-i(V_1+V_2))(t-s)} P_1 \approx & \int_s^t ds' \int_{s'}^t dt' P_2 e^{-iH(t-t')} \dot{P}_2 e^{-iH(t'-s')} \dot{P}_1 e^{-iH(s'-s)} P_1 \\ & \times \exp(-V_{20}(t-t') - V_{10}(s'-s))\end{aligned}\quad (3.28)$$

This expression is actually exact when the complex potential is absent, as is easily verified. Since \dot{P}_1 and \dot{P}_2 represent the fluxes at the boundary of Δ_1 and Δ_2 , one can easily identify the sections of the propagation which, semiclassically, are in Δ_1 , outside Δ_1 and Δ_2 , and in Δ_2 . The exponential suppression factors involving the complex potential for propagation inside Δ_1 and Δ_2 are inserted using a semiclassical approximation along the lines of Eq.(3.18). Inserting in Eq.(3.26), we thus obtain

$$\begin{aligned}
C_{\Delta_1\Delta_2} = & - \int_{-\infty}^{\infty} dt \int_{-\infty}^t ds \int_s^t ds' \int_{s'}^t dt' V_2(t) \dot{P}_2(t') \dot{P}_1(s') V_1(s) \\
& \times \exp(-V_{20}(t-t') - V_{10}(s'-s)) \\
& - \int_{-\infty}^{\infty} dt \int_{-\infty}^t ds \int_s^t ds' \int_{s'}^t dt' V_1(t) \dot{P}_1(t') \dot{P}_2(s') V_2(s) \\
& \times \exp(-V_{10}(t-t') - V_{20}(s'-s))
\end{aligned} \tag{3.29}$$

IV. PROPERTIES OF THE CLASS OPERATORS

We now examine the properties of the class operators Eq.(3.20), (3.29) and confirm that they give the desired results.

A. Single Region

It is easy to show that the class operator for a single region Eq.(3.20) has a sensible classical limit. Classically, $P(t)$ is a function on classical trajectories with $P(t) = 1$ when the classical trajectory is in Δ and is zero otherwise. Suppose a given trajectory $q^a(t)$ enters Δ at some stage in its history so intersects the boundary twice (recalling we have essentially assumed no more than two intersections in the semiclassical approximation Eq.(3.18)). For a given choice of parametrization of the trajectory, it enters Δ at parameter time t_a and leaves at time $t_b > t_a$ (see Figure 4). (We may parameterize it in the opposite direction, with the same ultimate result). Then the derivative of $P(s)$ is

$$\dot{P}(s) = \delta(s - t_a) - \delta(s - t_b) \tag{4.1}$$

and we have

$$C_{\Delta} = \int_{t_a}^{t_b} dt \int_{t_a}^t ds V_0 e^{-V_0(t-s)} [\delta(s - t_a) - \delta(s - t_b)] \tag{4.2}$$

Since $s \leq t \leq t_b$, the second δ -function in Eq.(4.2) makes no contribution to the integral. This is exactly the desired property – the expression for C_Δ registers only the first intersection of the trajectory with the boundary, but not the second intersection. The integral is easily evaluated with the result,

$$C_\Delta = 1 - e^{-V_0(t_b - t_a)} \quad (4.3)$$

This is approximately 1, as required, as long as

$$V_0(t_b - t_a) \gg 1 \quad (4.4)$$

We now give the broad picture in the quantum case and confirm some of the details in some simple models in the next section. Suppose we operate with C_Δ on an eigenstate $|\Psi_\lambda\rangle$ of H . The time integrals in Eq.(3.20) are easily carried out and the result is

$$C_\Delta |\Psi_\lambda\rangle = 2\pi V_0 \delta(H - \lambda) P G_V \dot{P} |\Psi_\lambda\rangle \quad (4.5)$$

where

$$G_V = \int_0^\infty dt e^{-i(H-\lambda)t - V_0 t} \quad (4.6)$$

$$= \frac{-i}{H - \lambda - iV_0} \quad (4.7)$$

and we have used

$$\delta(H - \lambda) = \frac{1}{2\pi} \int_{-\infty}^\infty dt e^{-i(H-\lambda)t} \quad (4.8)$$

The \dot{P} term is a current operator on the boundary Σ of Δ and may be written

$$\begin{aligned} \dot{P} &= i[H, P] \\ &= -\hat{p}_n \delta_\Sigma(\hat{q}) - \delta_\Sigma(\hat{q}) \hat{p}_n \end{aligned} \quad (4.9)$$

where

$$\delta_\Sigma(\hat{q}) = \int_\Sigma d^{n-1}q |q\rangle \langle q| \quad (4.10)$$

is a δ -function operator in the surface Σ and $\hat{p}_n = n^a \hat{p}_a$ is the component of the momentum operator normal to Σ with n^a the outward pointing normal. The normal n^a will depend on q in general so there may be an operator ordering issue in making \hat{p}_n hermitian. The difference between different ordering will involve a term of the form $\nabla_a n^a$, essentially the

extrinsic curvature of Σ , and this will be small if Δ is sufficiently large and its boundary reasonably smooth. Note that it is sometimes also convenient to write \dot{P} as

$$\dot{P} = i \int_{\Sigma} d^{n-1}q |q\rangle \overleftrightarrow{\partial}_n \langle q| \quad (4.11)$$

It is very useful to separate the current operator at the boundary into ingoing and outgoing parts according to the sign of \hat{p}_n at the boundary

$$\dot{P} = (\dot{P})_{in} - (\dot{P})_{out} \quad (4.12)$$

where $(\dot{P})_{in}$ consists of the components of \dot{P} with incoming momentum

$$(\dot{P})_{in} = -\hat{p}_n \theta(-\hat{p}_n) \delta_{\Sigma}(\hat{q}) - \delta_{\Sigma}(\hat{q}) \hat{p}_n \theta(-\hat{p}_n) \quad (4.13)$$

and similarly for $(\dot{P})_{out}$. Examples of these expressions in particular models will be given in the following sections. The restriction to positive or negative p_n means that it is generally difficult to express $(\dot{P})_{in}$ and $(\dot{P})_{out}$ in the form Eq.(4.11), involving the derivative $\hat{p}_n = -i\partial_n$, unless operating on a state (such as a WKB state) with simplifying properties. Note that these definitions require only that the local flux operator on a *given* surface can be split into ingoing and outgoing parts. To do so globally on a family of surfaces is generally impossible, essentially due to the problem of time, but fortunately this is not required here.

The quantity G_V has the form of a Feynman propagator, Eq.(1.22), with V_0 playing the role of the “ $i\epsilon$ prescription”, as long as V_0 is sufficiently small (in comparison to an appropriate energy scale contained in H , such as p_0 in the case of the Klein-Gordon equation). We therefore expect it to have properties similar to G_F , as described in Section 1D.

However, V_0 is not set to zero exactly and this in fact means that G_V has two properties not possessed by G_F . First, the non-zero V_0 produces a suppression for widely separated initial and final points. In a path integral representation of $G_V(q, q')$, the sum will be dominated by classical paths from q to q' , to which one may associate the total parameter time τ of the path. From the integral representation Eq.(4.6) it can be seen that G_V will have an overall exponential suppression factor of the form $\exp(-V_0\tau)$. Thus, propagation with G_V will suppress configurations q and q' connected by classical trajectories of parameter time duration of greater than $1/V_0$. Second, recalling that the class operator is closely related to the S -matrix for scattering off a complex potential there will be some reflection involved and this appears in properties of G_V – it will not exactly possess the Feynman properties of

propagating positive frequencies to the future negative frequencies to the past, but may, for example, propagate some positive frequencies to the past. However, this “non-Feynman” propagation will be small for sufficiently small V_0 , as we will see in the next section, so this possibility will be ignored.

These properties of G_V are crucial to understanding the properties of C_Δ . First note that

$$\langle q | PG_V \dot{P} | \Psi_\lambda \rangle = -i \int_\Sigma d^{n-1} q' f_\Delta(q) G_V(q, q') \overleftrightarrow{\partial}_n \Psi_\lambda(q') \quad (4.14)$$

In this expression the propagator $G_V(q, q')$ propagates from the boundary Σ to a point q on the interior. The fact that G_V is, approximately, a propagator of the Feynman type means two things. First, there will be initial and final points q, q' for which the propagator is very small (due to “propagation outside the lightcone”, discussed in Section 1D). Secondly, when it is not small, one would expect it to involve only *ingoing* modes at the boundary (to the extent that reflection is ignored). Hence the PG_V terms effectively restrict the current operator \dot{P} at the boundary to ingoing modes only – exactly the result we are looking for. We therefore replace \dot{P} , with the current operator $(\dot{P})_{in}$ involving ingoing modes only

$$C_\Delta | \Psi_\lambda \rangle = 2\pi V_0 \delta(H - \lambda) PG_V (\dot{P})_{in} | \Psi_\lambda \rangle \quad (4.15)$$

Now note that since the PG_V terms have done their job of selecting the ingoing modes, they may be eliminated. More precisely, we write $P = 1 - \bar{P}$, where \bar{P} is the projector onto the region outside Δ , and noting that that

$$V_0 \delta(H - \lambda) G_V = \delta(H - \lambda) \quad (4.16)$$

we find

$$\begin{aligned} C_\Delta | \Psi_\lambda \rangle &= 2\pi \delta(H - \lambda) (\dot{P})_{in} | \Psi_\lambda \rangle \\ &\quad - 2\pi \delta(H - \lambda) \bar{P} G_V (\dot{P})_{in} | \Psi_\lambda \rangle \end{aligned} \quad (4.17)$$

Consider the second term on the right-hand side. It consists of ingoing modes at the boundary of Δ propagated with G_V to a final point which is *outside* Δ . Semiclassically, this corresponds to paths which have to traverse the entire width of Δ , so if Δ is sufficiently large, this will take a long parameter time τ and, as discussed above, G_V will contain a suppression factor of $\exp(-V_0\tau)$ in comparison to the first term in Eq.(4.17). This is exactly

analogous to the suppression of the second term in the classical case, Eq.(4.3). We thus deduce that

$$C_\Delta|\Psi_\lambda\rangle \approx 2\pi\delta(H-\lambda)(\dot{P})_{in}|\Psi_\lambda\rangle \quad (4.18)$$

Note that the approximation leading to dropping the second term in Eq.(4.17) also ensures that the result is independent of V_0 , like the classical case in the appropriate limit. Eq.(4.18) is the main result of this section.

Eq.(4.18) may also be expressed in terms of $(\dot{P})_{out}$ defined in Eq.(4.12). To see this, note that, since $\dot{P} = i[H, P]$, we have

$$\delta(H-\lambda')\dot{P}|\Psi_\lambda\rangle = i(\lambda' - \lambda)\delta(H-\lambda')P|\Psi_\lambda\rangle \quad (4.19)$$

This is zero for $\lambda = \lambda'$, as long as $\langle\lambda|P|\lambda\rangle$ is well-defined, where $|\lambda\rangle$ are eigenstates of H . (It may not be well-defined if P projects onto an infinite region – see Appendix A). Eq.(4.12) then implies

$$\delta(H-\lambda)(\dot{P})_{in}|\Psi_\lambda\rangle = \delta(H-\lambda)(\dot{P})_{out}|\Psi_\lambda\rangle \quad (4.20)$$

so Eq.(4.18) may be expressed in terms of either the ingoing or outgoing flux or both.

It is also useful to note that the right-hand side of Eq.(4.18) may be written

$$2\pi\delta(H-\lambda)(\dot{P})_{in}|\Psi_\lambda\rangle = I_\Sigma|\Psi_\lambda\rangle \quad (4.21)$$

where

$$I_\Sigma = \int_{-\infty}^{\infty} dt e^{iHt}(\dot{P})_{in}e^{-iHt} \quad (4.22)$$

This is an intersection number operator for ingoing flux at the boundary Σ of Δ . Hence the class operator is essentially the intersection number I_Σ , and clearly commutes with H . It is classically equal to 1 for trajectories with ingoing flux at Σ (with no more than two intersections of the boundary, in the approximation we are using), and zero for trajectories not intersecting Σ . Of course, one may have guessed this approximate formula for the class operator, but a class operator is fundamentally defined as a product of projectors (or quasi-projectors) and the derivation given here makes it clear how this obvious guess arises from the fundamental definition. Note also the the class operator is hermitian in this case, so there is no need to consider the modified propagator Eq.(3.11).

The form Eq.(4.18) may be used to check for decoherence of histories in specific models and we will see this later. When there is decoherence of histories, the probabilities are given

by the average of a single class operator, Eq.(1.19), which in this case reads

$$\langle \Psi_{\lambda'} | C_{\Delta} | \Psi_{\lambda} \rangle = 2\pi \langle \Psi_{\lambda} | (\dot{P})_{in} | \Psi_{\lambda} \rangle \delta(\lambda - \lambda') \quad (4.23)$$

Following the induced inner product prescription, we drop the δ -function on the right and then set $\lambda = \lambda' = 0$, so the probability in terms of a solution $|\Psi\rangle$ of the Wheeler-DeWitt equation is

$$\langle \Psi | C_{\Delta} | \Psi \rangle_{phys} = 2\pi \langle \Psi | (\dot{P})_{in} | \Psi \rangle \quad (4.24)$$

This is essentially the ingoing Klein-Gordon flux on the boundary of Δ , as expected. (The factor of 2π relates to the induced inner product as described in Appendix A).

A more detailed calculation in a specific model is required to see that the above argument works. In particular, it is necessary to show that the various requirements on V_0 can be simultaneously met – it has to be small enough for G_V to function as a Feynman propagator and for reflection to be neglected, but large enough to ensure independence of V_0 and the dropping of the second term in Eq.(4.17). We will see in the models below that this is indeed possible.

B. Two Regions

We first consider the class operator Eq.(3.29) for two regions in the classical case. Suppose a classical trajectory enters Δ_1 at t_a , leaves at t_b , enters Δ_2 at t_c and leaves at t_d (with no more than two crossings of the boundaries of each region). See Figure 5. Then we have

$$\dot{P}_2(t') \dot{P}_1(s') = [\delta(t' - t_c) - \delta(t' - t_d)] [\delta(s' - t_a) - \delta(s' - t_b)] \quad (4.25)$$

It is easy to see that only one of the two terms in Eq.(3.29) contributes – the other term corresponds to the time-reversed trajectory. One can also see that the δ -functions at $t' = t_d$ and $s' = t_a$ make no contribution to the integral. Hence the only contribution comes from the time of departure t_b from Δ_1 and the time t_c of entering Δ_2 , clearly sufficient to characterize histories which spend time in both regions without overcounting. Evaluating the integral we find

$$C_{\Delta_1 \Delta_2} = (1 - e^{-V_{20}(t_d - t_c)}) (1 - e^{-V_{10}(t_b - t_a)}) \quad (4.26)$$

which is approximately 1, as required, as long as the trajectory spends sufficiently long in each region. For trajectories entering only one region, the \dot{P} term associated with the other

region is zero, so the class operator is zero. Classically, the class operator therefore has all the desired properties.

In the quantum case, we follow steps similar to the case for one region considered above. We consider the action of the class operator $C_{\Delta_1\Delta_2}$, defined in Eq.(3.29) on an eigenstate $|\Psi_\lambda\rangle$ of H . Changing variables from s, s', t' to

$$\begin{aligned}\bar{s} &= t - s \\ \bar{s}' &= s' - s \\ \bar{t}' &= t - t'\end{aligned}\tag{4.27}$$

the t integral may be done with the result

$$\begin{aligned}C_{\Delta_1\Delta_2}|\Psi_\lambda\rangle &= -2\pi \int_0^\infty d\bar{s} \int_0^{\bar{s}} d\bar{s}' \int_0^{\bar{s}-\bar{s}'} d\bar{t}' \exp(-V_{20}\bar{t}' - V_{10}\bar{s}') \\ &\times \delta(H - \lambda) V_2 e^{-iH\bar{t}'} \dot{P}_2 e^{-iH(\bar{s}-\bar{t}'-\bar{s}')} \dot{P}_1 e^{-iH\bar{s}'} V_1 |\Psi_\lambda\rangle e^{i\lambda\bar{s}} \\ &+ (1 \leftrightarrow 2)\end{aligned}\tag{4.28}$$

Now note that

$$\begin{aligned}\dot{P}_1 e^{-iH\bar{s}'} V_1 |\Psi_\lambda\rangle &\approx -V_{10}(\dot{P}_1)_{out} e^{-iH\bar{s}'} P_1 |\Psi_\lambda\rangle \\ &\approx -V_{10} e^{-i\lambda\bar{s}'} (\dot{P}_1)_{out} |\Psi_\lambda\rangle\end{aligned}\tag{4.29}$$

The first approximation arises because the combination $\dot{P}_1 \exp(-iH\bar{s}') P_1$ is propagation from inside Δ_1 to the boundary with only positive \bar{s}' , which means that there are only outgoing modes at the boundary. The second approximation arises because, once the restriction is made to outgoing modes, the projection P_1 may be dropped (similar to dropping the second term in Eq.(4.17)). Similar approximations may be made with the terms $\delta(H - \lambda) V_2 e^{-iH\bar{t}'} \dot{P}_2$. We thus obtain

$$\begin{aligned}C_{\Delta_1\Delta_2}|\Psi_\lambda\rangle &= 2\pi V_{10} V_{20} \int_0^\infty d\bar{s} \int_0^{\bar{s}} d\bar{s}' \int_0^{\bar{s}-\bar{s}'} d\bar{t}' \exp(-V_{20}\bar{t}' - V_{10}\bar{s}') \\ &\times \delta(H - \lambda) (\dot{P}_2)_{in} e^{-i(H-\lambda)(\bar{s}-\bar{t}'-\bar{s}')} (\dot{P}_1)_{out} |\Psi_\lambda\rangle \\ &+ (1 \leftrightarrow 2)\end{aligned}\tag{4.30}$$

The integrals may be carried out with the result,

$$C_{\Delta_1\Delta_2}|\Psi_\lambda\rangle = 2\pi\delta(H - \lambda) \left[(\dot{P}_2)_{in} G_F(\lambda) (\dot{P}_1)_{out} + (1 \leftrightarrow 2) \right] |\Psi_\lambda\rangle\tag{4.31}$$

where $G_F(\lambda)$ is the Feynman propagator at eigenvalue λ ,

$$\begin{aligned} G_F(\lambda) &= \int_0^\infty dt e^{-i(H-\lambda-i\epsilon)} \\ &= \frac{-i}{H-\lambda-i\epsilon} \end{aligned} \quad (4.32)$$

We may again attempt to interchange ingoing and outgoing flux operators, along the lines of Eq.(4.20). However, since

$$(H-\lambda)G_F(\lambda) = -i \quad (4.33)$$

there are extra terms of the form $(\dot{P}_2)_{in}P_1$ and $(\dot{P}_1)_{in}P_2$, but these are zero since they are products of operators localized about spatially distinct regions. We thus find

$$C_{\Delta_1\Delta_2}|\Psi_\lambda\rangle = 2\pi\delta(H-\lambda) \left[(\dot{P}_2)_{in}G_F(\lambda)(\dot{P}_1)_{in} + (1 \leftrightarrow 2) \right] |\Psi_\lambda\rangle \quad (4.34)$$

(or equivalently in terms of outgoing flux).

At this stage it is of interest to examine the difference between this propagator and the modified version, Eq.(3.11), invariant under reversals of parameter time, since the presence of $G_F(\lambda)$ in Eq.(4.34) rather than $\delta(H-\lambda)$ means that it is not invariant. It is easy to see that the modification Eq.(3.11) effectively produces the replacement

$$G_F(\lambda) \rightarrow \frac{1}{2} \left(G_F(\lambda) + G_F^\dagger(\lambda) \right) = \frac{1}{2} (2\pi) \delta(H-\lambda) \quad (4.35)$$

and we obtain for the modified propagator

$$\begin{aligned} C'_{\Delta_1\Delta_2}|\Psi_\lambda\rangle &= \frac{1}{2} (2\pi)^2 \delta(H-\lambda) (\dot{P}_2)_{in} \delta(H-\lambda) (\dot{P}_1)_{in} |\Psi_\lambda\rangle \\ &+ \frac{1}{2} (2\pi)^2 \delta(H-\lambda) (\dot{P}_1)_{in} \delta(H-\lambda) (\dot{P}_2)_{in} |\Psi_\lambda\rangle \end{aligned} \quad (4.36)$$

This result may also be expressed in terms of intersection number operators,

$$C'_{\Delta_1\Delta_2} = \frac{1}{2} (I_{\Sigma_2} I_{\Sigma_1} + I_{\Sigma_1} I_{\Sigma_2}) \quad (4.37)$$

It is now easy to guess the form of the class operator for n regions. It is,

$$C'_n = \frac{1}{n!} (I_{\Sigma_1} I_{\Sigma_2} \cdots I_{\Sigma_n} + \text{permutations}) \quad (4.38)$$

where “permutations” means add all possible permutations of the n regions, to give a total of $n!$ terms. This final result has a particularly natural form which also suggests that it may have simple path integral representations. This will be explored elsewhere. (See also Ref.[41] for similar expressions, derived using a detector model for quantum cosmology).

V. SOME SIMPLE EXAMPLES

To verify the properties of the class operator C_Δ outlined above, we compute it explicitly in some simple examples. We first consider a one-dimensional example.

A. A One-Dimensional Example

We take the Hamiltonian to be the free particle Hamiltonian $H = p^2/2m$ and the region Δ to be the interval $[-L, L]$. We take the initial state to be an energy eigenstate

$$\langle x|p\rangle = \frac{1}{(2\pi)^{1/2}} e^{ipx} \quad (5.1)$$

with $p > 0$ and energy $E = p^2/2m$. (In this case, unlike the Wheeler-DeWitt and Klein-Gordon equations, the eigenvalue of H is the physical energy, so we do not take $E = 0$ at the end of the calculation. However, the inner products are still regularized by taking different values of E on either side of any inner product.)

Our aim is to confirm in this example the properties of the class operator Eq.(4.5), which in this case we write as,

$$C_\Delta|p\rangle = 2\pi V_0 \delta(H - E) P G_V \dot{P}|p\rangle \quad (5.2)$$

P is the projection operator onto the region $[-L, L]$ and may also be represented in terms of the region's characteristic function $f_L(x)$, so $P = f_L(\hat{x})$. It follows that

$$\dot{P} = \frac{1}{2m} [\hat{p}\delta(\hat{x} + L) + \delta(\hat{x} + L)\hat{p} - \hat{p}\delta(\hat{x} - L) - \delta(\hat{x} - L)\hat{p}] \quad (5.3)$$

For the $p > 0$ initial state considered here, we identify the first two terms, at $x = -L$, as $(\dot{P})_{in}$ and the last two terms, at $x = L$, as $-(\dot{P})_{out}$,

$$\dot{P} = (\dot{P})_{in} - (\dot{P})_{out} \quad (5.4)$$

We may now write

$$\begin{aligned} \langle x|P G_V \dot{P}|p\rangle &= \int dy G_V(x, y) \langle y|\dot{P}|p\rangle \\ &= \frac{-i}{2m\sqrt{2\pi}} f_L(x) \left(\left[G_V(x, y) \overleftrightarrow{\partial}_y e^{ipy} \right]_{y=-L} - \left[G_V(x, y) \overleftrightarrow{\partial}_y e^{ipy} \right]_{y=L} \right) \end{aligned} \quad (5.5)$$

The Green function may be calculated explicitly using the form Eq.(4.6), which may be written

$$G_V(x, y) = \int_0^\infty dt \left(\frac{m}{2\pi i t} \right)^{1/2} \exp \left(im \frac{(x - y)^2}{2t} + i(E + iV_0)t \right) \quad (5.6)$$

The integral may be carried out explicitly [42], with the result

$$G_V(x, y) = \frac{m}{Q} [\theta(x - y)e^{i(x-y)Q} + \theta(y - x)e^{-i(x-y)Q}] \quad (5.7)$$

where we have introduced the complex momentum

$$Q = \sqrt{2m(E + iV_0)} \quad (5.8)$$

The interesting case is that in which $V_0 \ll E$ (which is the condition for negligible reflection in the scattering off the complex potential) and we can then expand

$$\begin{aligned} Q &= \sqrt{2mE} \left(1 + i\frac{V_0}{E}\right)^{1/2} \\ &= p + i\frac{V_0m}{p} + \dots \end{aligned} \quad (5.9)$$

where $p = \sqrt{2mE}$. This means that the Green function has the form

$$G_V(x, y) \approx \frac{m}{p} [\theta(x - y)e^{i(x-y)p} + \theta(y - x)e^{-i(x-y)p}] \exp\left(-\frac{V_0m}{p}|x - y|\right) \quad (5.10)$$

It therefore has the form of Feynman type Green function, but there is also exponential suppression for large separations of initial and final points, as anticipated.

To evaluate Eq.(5.5), we consider the action of the Green function G_V on a plane wave state $|p\rangle$ with $p > 0$. We have

$$\begin{aligned} \frac{-i}{2m} G_V(x, y) \overleftrightarrow{\partial}_y e^{ipy} &= \theta(x - y) \frac{(Q + p)}{2Q} \exp(ipx + i(x - y)(Q - p)) \\ &\quad - \theta(y - x) \frac{(Q - p)}{2Q} \exp(-ipx + 2ipy + i(y - x)(Q - p)) \end{aligned} \quad (5.11)$$

For $E \gg V_0$, this has the approximate form,

$$\begin{aligned} \frac{-i}{2m} G_V(x, y) \overleftrightarrow{\partial}_y e^{ipy} &= \theta(x - y) e^{ipx} \exp\left(-\frac{V_0m}{p}|x - y|\right) \\ &\quad - 4i\frac{V_0}{E}\theta(y - x) e^{-ipx+2ipy} \exp\left(-\frac{V_0m}{p}|x - y|\right) \end{aligned} \quad (5.12)$$

The first term corresponds to the familiar property of consisting of positive momentum for $x > y$ (with the exponential suppression factor mentioned above). The second term is not a familiar property of the Feynman Green function since it corresponds to negative momentum for $x < y$ (which we do not expect since the incoming state consists only of

positive momentum). This actually corresponds to reflection, and this term will be small for $V_0 \ll E$, which we assume.

These results show that the second term in Eq.(5.5), the term corresponding to $(\dot{P})_{out}$ may be dropped, as expected. We have now confirmed that

$$C_\Delta|p\rangle \approx 2\pi V_0 \delta(H - E) P G_V(\dot{P})_{in}|p\rangle \quad (5.13)$$

Following the general discussion of Section 4, we write $P = 1 - \bar{P}$ and obtain

$$\begin{aligned} C_\Delta|p\rangle &\approx 2\pi \delta(H - E) (\dot{P})_{in}|p\rangle \\ &- 2\pi V_0 \delta(H - E) \bar{P} G_V(\dot{P})_{in}|p\rangle \end{aligned} \quad (5.14)$$

We need to show that the second term is small. We have

$$\langle x | \bar{P} G_V(\dot{P})_{in} | p \rangle = \frac{-i}{2m\sqrt{2\pi}} \bar{f}_L(x) \left[G_V(x, y) \overleftrightarrow{\partial}_y e^{ipy} \right]_{y=-L} \quad (5.15)$$

where $\bar{f}_L(x)$ is the characteristic function for the region outside Δ , so $x \geq L$ and $x \leq -L$. The properties of G_V deduce above confirm that this expression is small. For $x \geq L$, there is exponential suppression of the Green function since $|x - y| \geq 2L$. The exponential suppression is of order $\exp(-V_0\tau)$, where

$$\tau = \frac{2mL}{p} \quad (5.16)$$

which is the time for a classical trajectory to traverse Δ . On the other hand, values of $x \leq -L$ can only be reached by reflection, and this is small since $V_0 \ll E$.

We have therefore confirmed the desired result that the class operator has the form

$$C_\Delta|p\rangle \approx 2\pi \delta(H - E) (\dot{P})_{in}|p\rangle \quad (5.17)$$

and this result is valid in the regime

$$\frac{1}{\tau} \ll V_0 \ll E \quad (5.18)$$

(This regime is a commonly encountered one in studies of the arrival time in non-relativistic quantum mechanics [29, 31]). The outer parts of the inequality imply that $E\tau \gg 1$, or equivalently,

$$pL \gg 1 \quad (5.19)$$

which is easily satisfied for sufficiently large L and p . It is essentially the condition that the size of Δ is much greater than the wavelength of the quantum state.

Since

$$2\pi\delta(H - E) = G_F + G_F^\dagger \quad (5.20)$$

(where G_F is the Feynman Green function, obtained from G_V by letter $V_0 \rightarrow 0+$), we have

$$\langle x|\delta(H - E)|y\rangle = \frac{2\pi m}{p} (e^{ip(x-y)} + e^{-ip(x-y)}) \quad (5.21)$$

and it follows that Eq.(5.17) may be evaluated with the trivial result

$$C_\Delta|p\rangle \approx |p\rangle \quad (5.22)$$

This is completely expected since every plane wave enters the region Δ .

However, for the class operator operating on the initial state Eq.(5.17) to have a more interesting and non-trivial form, we need to look at a two-dimensional example. This will be useful for the purposes of examining the decoherence properties of some simple states.

B. A Two-Dimensional Example

We again take a free particle but in two dimensions, with Hamiltonian $H = (p_1^2 + p_2^2)/2m$, and we take the region Δ to be a rectangle of sides $2L_1$ and $2L_2$ centered at the origin. We use coordinates x_1, x_2 and the characteristic function of Δ is

$$f_\Delta(x_1, x_2) = f_{L_1}(x_1)f_{L_2}(x_2) \quad (5.23)$$

We take the initial state $|\Psi\rangle$ to be a plane wave in the 1-direction, $e^{ip_1x_1}$, with $p_1 > 0$, so there is no momentum in the 2-direction. The analysis of the one-dimensional example may be used to show, very easily, that the class operator is again of the form Eq.(5.17), with

$$(\dot{P})_{in} = \frac{1}{2m} [\hat{p}_1\delta(\hat{x}_1 + L_1) + \delta(\hat{x}_1 + L_1)\hat{p}_1] f_{L_2}(\hat{x}_2) \quad (5.24)$$

Denoting the matrix elements of $\delta(H - E)$ by $G(\mathbf{x}|\mathbf{y})$, we have

$$\begin{aligned} \langle \mathbf{x}|C_\Delta|\Psi\rangle &= 2\pi\langle x_1, x_2|\delta(H - E)(\dot{P})_{in}|\Psi\rangle \\ &= \frac{-i\sqrt{2\pi}}{2m} \int_{-L_2}^{L_2} dy_2 \left[G(x_1, x_2|y_1, y_2) \overleftrightarrow{\partial}_{y_1} e^{ip_1y_1} \right]_{y_1=-L_1} \end{aligned} \quad (5.25)$$

Note that, due to the suppression effect in G_V , the spatial size $2L_1$ of Δ in the x_1 -direction has essentially dropped out of the expression for the class operator and it is expressed now only in terms of the incoming flux at $x_1 = -L$.

Eq.(5.25) may be approximately calculated, at some length, but the form of the result for $C_\Delta|\Psi\rangle$ is easy to anticipate on general physical grounds. We still have the result Eq.(5.20), so we first consider the action of G_F attached to the initial state as in Eq.(5.25). The physical situation therefore consists of an incoming plane wave $\exp(ip_1x_1)$ from $x_1 < 0$ encountering a gate of width $2L_2$ in the x_2 direction located at $x_1 = -L$. This situation is very similar to the Mott analysis of the particle detection in a cloud chamber [41, 43]. The localization by the gate to spatial width $2L_2$ produces a momentum uncertainty in the 2-direction Δp_2 of order $1/L_2$. Since the momentum in the 1-direction is p_1 , it is easy to see that this produces a spreading in $x_1 > 0$ of angular size of order $1/(p_1L_2)$. This will be very small for sufficiently large L_2 . If we now consider also the action of G_F^\dagger on the same initial state, it produces essentially the same effect in $x_1 < 0$.

The final result is therefore that $C_\Delta|\Psi\rangle$ consists of a plane wave $\exp(ip_1x_1)$ localized on a tube of width $2L_2$ around the x_1 -axis, with the tube opening out by a small angle $1/(p_1L_1)$ as $x_1 \rightarrow \pm\infty$. See Figure 6. To the extent that the angular spreading can be ignored, the result has the very approximate form

$$\langle x_1, x_2 | C_\Delta | \Psi \rangle \approx e^{ip_1x_1} f'_{L_2}(x_2) \quad (5.26)$$

where f'_{L_2} is a function localized to a width L_2 around the origin (not necessarily the same as the exact window function used above).

This approximate result may be used to address the decoherence properties of the initial state $|\Psi\rangle$ defined above. The class operator for not entering Δ is clearly

$$\langle x_1, x_2 | \bar{C}_\Delta | \Psi \rangle \approx e^{ip_1x_1} \bar{f}'_{L_2}(x_2) \quad (5.27)$$

where $\bar{f}'_{L_2} = 1 - f'_{L_2}$, so $\bar{C}_\Delta|\Psi\rangle$ is localized outside the tube defined in Eq.(5.26). We immediately see that

$$\langle \Psi | \bar{C}_\Delta C_\Delta | \Psi \rangle \approx 0 \quad (5.28)$$

quite simply because the two class operators are spatially localized about different non-overlapping regions. There is therefore approximate decoherence of histories in this case.

Another interesting case is to take the same region Δ but take a superposition of initial states

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|\Psi_1\rangle + |\Psi_2\rangle) \quad (5.29)$$

where $|\Psi_1\rangle$ is a plane wave in the 1-direction, $\exp(ip_1x_1)$, considered above, and $|\Psi_2\rangle$ is a plane wave in the 2-direction, $\exp(ip_2x_2)$. Each state individually produces decoherence of histories, as shown above, but there will be cross terms in the decoherence functional,

$$\langle\Psi|\bar{C}_\Delta C_\Delta|\Psi\rangle \approx \frac{1}{2}\langle\Psi_2|\bar{C}_\Delta C_\Delta|\Psi_1\rangle + \frac{1}{2}\langle\Psi_1|\bar{C}_\Delta C_\Delta|\Psi_2\rangle \quad (5.30)$$

The first term is approximately,

$$\langle\Psi_2|\bar{C}_\Delta C_\Delta|\Psi_1\rangle \approx \int dx_1 dx_2 f'_{L_2}(x_2) f_{L_1}(x_1) \exp(ip_1x_1 + ip_2x_2) \quad (5.31)$$

It is easy to see that this expression will be very small as long as $p_1L_1 \gg 1$ and $p_2L_2 \gg 1$, due to averaging out of oscillations. There will therefore be decoherence of superposition states as long as the region Δ is sufficiently large.

The essential reason for decoherence in this case is that the orthogonality of $|\Psi_1\rangle$ and $|\Psi_2\rangle$ is little disturbed by the action of the class operators as long as Δ is large enough. (Recall that interference effects in the double slit experiment will only arise for narrow slits very close together). For regions Δ of small size, it may be necessary to consider coupling to an environment to produce decoherence of histories. This will not be explored here.

C. The Klein-Gordon Equation and the Probability for Surface Crossing

We now consider the problem of assigning probabilities to histories of the relativistic particle in flat space which cross or do not cross the spacelike surface $x_0 = 0$ in the spatial region Σ . This is slightly different to the cases considered so far since we need to show exactly how the results derived above for entering regions Δ may be used to derive probabilities for crossing surfaces. This example also involves the effects of the signature of the metric. A decoherent histories analysis of the Klein-Gordon system was given in detail in Ref.[10], but it encountered difficulties in definition of the class operators. A somewhat heuristic definition was used, with satisfactory physical results, but the underlying origin of this definition was not clear. Here, we show how this heuristic definition arises from the more rigorous definitions used in this paper.

To define a class operator for crossing the spacelike surface Σ , we regard the surface as part of the boundary of a spacetime region Δ . For simplicity we take the three-dimensional region Σ to be the interior of a 2-sphere at $x^0 = 0$. We then define Δ by requiring that it is a null cone in $x^0 > 0$ with Σ its base. (A two-dimensional version of this is depicted in Figure 7). The class operator is again given by Eq.(4.18), with $|\Psi\rangle$ a solution to the Klein-Gordon equation which may contain positive and negative frequencies,

$$\Psi = \Psi^+ + \Psi^- \quad (5.32)$$

The flux operator $(\dot{P})_{in}$ consists of contributions from the two parts of the boundary of Δ ,

$$(\dot{P})_{in} = (\dot{P})_{in}^{\Sigma} + (\dot{P})_{in}^{cone} \quad (5.33)$$

The flux operator on Σ is clearly just the positive frequency flux at this boundary

$$(\dot{P})_{in}^{\Sigma} = (\theta(\hat{p}_0)\hat{p}_0\delta(\hat{x}^0) + \delta(\hat{x}^0)\theta(\hat{p}_0)\hat{p}_0) f_{\Sigma}(\hat{x}^i) \quad (5.34)$$

where $f_{\Sigma}(x^i)$ is a window function localized in Σ . The remaining part of the flux operator describes the incoming flux on the null cone. Classically, since this surfaces is null, every incoming trajectory crossing the cone will cross Σ . An analogous result is approximately true in the quantum case, since propagation outside the lightcone is suppressed. Hence, these flux operators are approximately equal to the negative frequency flux at Σ ,

$$(\dot{P})_{in}^{cone} \approx (\theta(-\hat{p}_0)\hat{p}_0\delta(\hat{x}^0) + \delta(\hat{x}^0)\theta(-\hat{p}_0)\hat{p}_0) f_{\Sigma}(\hat{x}^i) \quad (5.35)$$

The class operator involves contributions from boths of these terms and may be written

$$C_{\Sigma}|\Psi_{\lambda}\rangle = 2\pi\delta(H - \lambda) (|\hat{p}_0|\delta(\hat{x}^0) + \delta(\hat{x}^0)|\hat{p}_0|) f_{\Sigma}(\hat{x}^i)|\Psi_{\lambda}\rangle \quad (5.36)$$

Noting that $\langle x|\delta(H)|y\rangle$ is the same as the the Klein-Gordon propagator $G^{(1)} = G^+ + G^-$ (where G^{\pm} are the positive and negative frequency Wightman functions [10]), we have, setting $\lambda = 0$,

$$\langle x|C_{\Sigma}|\Psi\rangle = 2\pi i \int_{\Sigma} d^3y \left[G^{(1)}(x, y) \overleftrightarrow{\partial}_0 \Psi^+(y) - G^{(1)}(x, y) \overleftrightarrow{\partial}_0 \Psi^-(y) \right] \quad (5.37)$$

This agrees with the definition in Ref.[10]. It consists of the initial state attached to $G^{(1)}$ with a “sign-adjusted” Klein-Gordon inner product to take care of the negative frequencies. It was shown in Ref.[10] that there is approximate decoherence between histories which cross

$x^0 = 0$ in Σ or outside Σ , again because propagation outside the lightcone is suppressed. The resulting probability for crossing is

$$p(\Sigma) = 2\pi i \int_{\Sigma} d^3x \left[\Psi^+(x) \overleftrightarrow{\partial}_0 \Psi^+(x) - \Psi^-(x) \overleftrightarrow{\partial}_0 \Psi^-(x) \right] \quad (5.38)$$

This is the expected result and is positive.

Hence, the decoherent histories approach described in this paper yields the expected results for the Klein-Gordon equation, improving on the heuristic analysis of Ref.[10]. Note that the method used above to relate probabilities for surface crossings to probabilities for entering regions is specific to the dynamics of the relativistic particle in flat space. More complicated systems will require a modified approach adapted to their particular dynamics.

VI. WKB REGIME

The most important case in which to check the ideas developed above is in the WKB regime. In the oscillatory regime, the solutions to the Wheeler-DeWitt equation have the form

$$\Psi = R e^{iS} \quad (6.1)$$

where R and S obey Eqs.(1.24), (1.25) as described earlier. More generally, the wave function is a superposition of WKB wave functions but we consider first the case of a single term. The heuristic interpretation of such states was described in Section 1D. Our aim is to show that the decoherent histories analysis reproduces the heuristic scheme. WKB states are locally plane wave states of the type considered in the previous Section, so we will appeal to that analysis to understand the properties WKB states.

We consider the action of the class operator for a single region Δ on a WKB state. We first consider the class operator Eq.(4.18) acting on WKB state (regularized by making it an eigenstate of H with eigenvalue λ)

$$\begin{aligned} \langle q | C_{\Delta} | \Psi_{\lambda} \rangle &= 2\pi \langle q | \delta(H - \lambda) (\dot{P})_{in} | \Psi_{\lambda} \rangle \\ &= 2\pi i \int_{\Sigma_{in}} d^{n-1}q' \langle q | \delta(H - \lambda) | q' \rangle \overleftrightarrow{\partial}_n \Psi_{\lambda}(q') \end{aligned} \quad (6.2)$$

Here Σ_{in} denotes the sections of the boundary where the flux is ingoing,

$$n \cdot \nabla S < 0 \quad (6.3)$$

where n^a is the outward pointing normal. The key property of the WKB wave function $\Psi_\lambda(q')$ is that it has momentum $p = \nabla S(q')$ at each point q' on the boundary. When the operator $\delta(H - \lambda)$ is applied, from the representation Eq.(4.8), we see that it's effect is to evolve the state $\Psi_\lambda(q')$ (restricted to Σ_{in}) forwards and backwards in parameter time, and then integrates over all times. Semiclassically, the evolution of the state $\Psi_\lambda(q')$ will be concentrated along the classical trajectories defined by initial positions q' in Σ_{in} and momenta $p = \nabla S(q')$, with some spreading of the wave packet, but this will be small if Δ is reasonably large. (This is analogous to the model of Section 5B).

We thus see the following: the wave function $\langle q|C_\Delta|\Psi_\lambda\rangle$ in Eq.(6.2) is spatially localized around the tube of classical trajectories passing through Δ with momenta $p = \nabla S$ (depicted in Figure 2). This may be approximately written in the alternative form

$$\langle q^a|C_\Delta|\Psi_\lambda\rangle \approx \theta(\tau_\Delta - \epsilon) Re^{iS} \quad (6.4)$$

where $\epsilon > 0$ is a small parameter to regularize the θ -function at zero argument. Here, $\tau_\Delta(q)$ is the parameter time spent by the classical trajectory $q_{cl}(t)$ (with initial value q and momentum $p = \nabla S(q)$) in the region Δ and may be written

$$\tau_\Delta(q) = \int_{-\infty}^{\infty} dt f_\Delta(q_{cl}(t)) \quad (6.5)$$

This has the property that

$$\nabla S \cdot \nabla \tau_\Delta = 0 \quad (6.6)$$

since $\nabla S \cdot \nabla$ simply translates along the classical trajectories. It follows from Eq.(1.25) that Eq.(6.4) is in fact a WKB solution to the Wheeler-DeWitt equation, since the θ -function essentially modifies the prefactor R but in a way that it still satisfies Eq.(1.25). (Of course, this is expected because C_Δ commutes with H).

Eq.(6.4) is a very useful result and allows us to check for decoherence very easily. The action of the class operator for not entering Δ is clearly

$$\langle q^a|\bar{C}_\Delta|\Psi_\lambda\rangle \approx \theta(\epsilon - \tau_\Delta) Re^{iS} \quad (6.7)$$

which is a WKB state localized on the set of trajectories not entering Δ . It immediately follows that

$$\langle \Psi_{\lambda'}|\bar{C}_\Delta C_\Delta|\Psi_\lambda\rangle \approx 0 \quad (6.8)$$

since the two states Eqs.(6.4), (6.7) are localized about complementary regions. There is therefore approximate decoherence of histories for a single WKB packet and for histories entering or not entering a single region Δ , as long as Δ is sufficiently large.

The key reason for the decoherence with a single WKB packet is related to the approximate determinism of the WKB wave functions: fixing values of position to lie on Σ_{in} also fixes the momenta, since $p = \nabla S$, so that Eq.(6.2) is concentrated along a tube of classical trajectories.

More generally, the initial state will be a superposition of WKB wave packets,

$$\Psi = \sum_k R_k e^{iS_k} \quad (6.9)$$

The component states in this sum are typically approximately orthogonal to each other as long as the phases S_k are sufficiently different. (This will depend on the detailed dynamics of the model). Following the analogous example in the simple models of Section 5B, we would expect that the class operators will not disturb the approximate orthogonality of these states as long as the region Δ is sufficiently large – again we expect the cross terms in the decoherence functional to average to zero because of oscillations, as in Eq.(5.30). Therefore, superpositions may in practice be treated as mixtures at sufficiently coarse-grained scales. Note that this statement also applies the special state,

$$\Psi = R (e^{iS} + e^{-iS}) \quad (6.10)$$

which arises from the Hartle-Hawking “no boundary” proposal [44]. That is, the interference between the two terms may be neglected.

Given decoherence, the probabilities are given by the general expression Eq.(4.24). It then follows that the probabilities for entering Δ coincide with Eq.(1.29), the sought-after result.

Now consider the case of probabilities for histories entering two regions, as described by the (modified) class operator Eq.(4.36). Since the two-region class operator is a sum of products of one-region class operators, its effect on the WKB wave functions is easy to see. The action of a single class operator gives Eq.(6.4). But since this is still a wave function of the WKB type, the action of a second class operator yields

$$\langle q^a | C_{\Delta_1 \Delta_2} | \Psi_\lambda \rangle \approx \theta(\tau_{\Delta_1} - \epsilon) \theta(\tau_{\Delta_2} - \epsilon) R e^{iS} \quad (6.11)$$

That is, it is a WKB wave function but restricted in such a way that its flux passes through both regions. See Figure 8. (It is easy to see that in this case the action of the unmodified class operator Eq.(4.34) is the same.) It is again easy to see that there is decoherence of histories and the probability is given by an expression of the form Eq.(1.29), but with the integral over the subset of incoming flux at Δ_1 which goes on to intersect Δ_2 .

From the above observations one can also see why the exponential WKB wave functions will *not* lead to decoherence of histories. The exponential wave functions have the form

$$\Psi = R e^{-I} \tag{6.12}$$

where I is real. The key difference between states of this type and the oscillatory type Eq.(6.1) is that they do not have a correlation between positions and momenta [28]. One would therefore expect the evolution of the state Eq.(6.2) to be spread all over the configuration space and not concentrated around a particular region. That is, these states do not have the approximate determinism of the oscillatory states. The states $C_\Delta|\Psi\rangle$ and $\bar{C}_\Delta|\Psi\rangle$ would then not be approximately orthogonal so there will be no decoherence of histories.

The decoherence of histories described here has arisen because of the approximate determinism of the oscillatory WKB states, together with the approximate orthogonality properties that arise when the regions Δ are sufficiently large. At finer grained scales, decoherence of histories may only be possible in more complicated models in which there is an environment of some sort. Models along these lines, in more basic approaches to quantum cosmology, have been considered previously [45], and one might expect that they may be adapted to the decoherent histories approach to quantum cosmology. (See also Ref.[11]).

In summary, we have derived from the decoherent histories approach the probabilities normally used in the heuristic WKB interpretation. To address these issues in more detail will require more specific quantum cosmological models. This will be considered elsewhere.

VII. DISCUSSION AND FURTHER ISSUES

We have presented a properly defined quantization procedure for quantum cosmology using the decoherent histories approach to quantum theory and derived from this the frequently used but heuristic WKB interpretation, involving fluxes of the WKB wave function.

The key idea was to use a complex potential to define the class operators for not entering a

region of configuration space. This method is adequately justified by its successful use in the arrival time problem in non-relativistic quantum theory. We showed that the class operators defined in this way have all the desired properties – they have the correct classical limit, are compatible with the constraint equation, and do not have difficulties with the Zeno effect. In a semiclassical approximation, they have an appealing form in terms of intersection number operators. They give sensible results in simple models and there is approximate decoherence of histories for certain types of initial state at sufficiently coarse grained scales.

Future papers will address the more detailed application of this approach to specific models and will also undertake a comparison of the decoherent histories approach described here to other approaches [5].

VIII. ACKNOWLEDGEMENTS

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APPENDIX A: OPERATORS AND INNER PRODUCTS FOR THE KLEIN-GORDON EQUATION

In this appendix we outline the relationship between the induced inner product and Klein-Gordon inner product. This has been described elsewhere (see, for example, Ref.[9]), but the derivation given here is different and will help give some insight into the form of some of the results of Section 4.

We use $x^\mu = (x^0, \mathbf{x})$ to denote spatial coordinates and take the signature of spacetime to be $(-+++)$. The Hamiltonian for the Klein-Gordon system is

$$H = -p_0^2 + \mathbf{p}^2 + m^2 \tag{A1}$$

The induced inner product begins by looking at eigenfunctions of H with eigenvalue λ , which we write as

$$\begin{aligned} \langle x | \lambda \mathbf{p} s \rangle &= \Psi_{\lambda \mathbf{p} s}(x) \\ &= N e^{i s p \cdot x} \end{aligned} \tag{A2}$$

where $p_0 = \sqrt{\mathbf{p}^2 + m^2 - \lambda}$ and $s = \pm 1$ labels the solutions as positive or negative frequency. We work with three different inner products. The first is the standard Schrödinger inner product,

$$\langle \lambda \mathbf{p} s | \lambda' \mathbf{p}' s' \rangle = \int d^4 x \Psi_{\lambda \mathbf{p} s}^*(x) \Psi_{\lambda' \mathbf{p}' s'}(x) \quad (\text{A3})$$

and the eigenfunctions are normalized with this inner product according to

$$\langle \lambda \mathbf{p} s | \lambda' \mathbf{p}' s' \rangle = \delta(\lambda - \lambda') \delta(\mathbf{p} - \mathbf{p}') \delta_{ss'} \quad (\text{A4})$$

The goal is to relate this to the Klein-Gordon inner product Eq.(1.6). One way to do this is to integrate out x^0 in Eq.(A3), but here we proceed differently.

We introduce the projection operator $P = \theta(\hat{x}^0)$ onto $x^0 > 0$ and consider the current operator

$$\hat{J} = \int_{-\infty}^{\infty} dt \dot{P}(t) \quad (\text{A5})$$

On the one hand, we can carry out the integral with the result

$$\begin{aligned} \hat{J} &= [\theta(\hat{x}^0 + 2\hat{p}^0 t)]_{t=-\infty}^{t=\infty} \\ &= \epsilon(\hat{p}^0) \end{aligned} \quad (\text{A6})$$

where $\epsilon(\hat{p}^0)$ is the signum function operator. On the other hand, we can differentiate P with the result

$$\begin{aligned} \dot{P}(t) &= i[H, \theta(\hat{x}^0)] \\ &= \hat{p}^0 \delta(\hat{x}^0) + \delta(\hat{x}^0) \hat{p}^0 \end{aligned} \quad (\text{A7})$$

so that

$$\hat{J} = \int_{-\infty}^{\infty} dt e^{iHt} (\hat{p}^0 \delta(\hat{x}^0) + \delta(\hat{x}^0) \hat{p}^0) e^{-iHt} \quad (\text{A8})$$

We now insert the identity

$$\epsilon(\hat{p}^0) \hat{J} = 1 \quad (\text{A9})$$

with \hat{J} given by Eq.(A8) in the inner product Eq.(A4), with the result

$$\begin{aligned} \langle \lambda \mathbf{p} s | \lambda' \mathbf{p}' s' \rangle &= \langle \lambda \mathbf{p} s | \epsilon(\hat{p}^0) \hat{J} | \lambda' \mathbf{p}' s' \rangle \\ &= 2\pi \delta(\lambda - \lambda') s \langle \lambda \mathbf{p} s | (\hat{p}^0 \delta(\hat{x}^0) + \delta(\hat{x}^0) \hat{p}^0) | \lambda' \mathbf{p}' s' \rangle \end{aligned} \quad (\text{A10})$$

We now identify the inner product expression on the right-hand side as the Klein-Gordon inner product between states with the same λ ,

$$\begin{aligned} (\Psi_{\lambda \mathbf{p}s}, \Psi_{\lambda \mathbf{p}'s'})_{KG} &\equiv \langle \lambda \mathbf{p}s | (\hat{p}^0 \delta(\hat{x}^0) + \delta(\hat{x}^0) \hat{p}^0) | \lambda \mathbf{p}'s' \rangle \\ &= i \int_{x^0=0} d^3x \Psi_{\lambda \mathbf{p}s}^*(x) \overleftrightarrow{\partial}_0 \Psi_{\lambda \mathbf{p}'s'}(x) \end{aligned} \quad (\text{A11})$$

(where $\hat{p}^0 = -\hat{p}_0 = i\partial_0$). Therefore the relationship between the Schrödinger inner product and Klein-Gordon inner product is

$$\langle \lambda \mathbf{p}s | \lambda' \mathbf{p}'s' \rangle = 2\pi \delta(\lambda - \lambda') s (\Psi_{\lambda \mathbf{p}s}, \Psi_{\lambda \mathbf{p}'s'})_{KG} \quad (\text{A12})$$

Finally, the induced (or physical) inner product on eigenstates with the same λ , is defined as outlined in Section 1, essentially by factoring out the δ -function

$$\langle \lambda \mathbf{p}s | \lambda' \mathbf{p}'s' \rangle = \delta(\lambda - \lambda') \langle \lambda \mathbf{p}s | \lambda \mathbf{p}'s' \rangle_{phys} \quad (\text{A13})$$

so we deduce that

$$\langle \lambda \mathbf{p}s | \lambda \mathbf{p}'s' \rangle_{phys} = 2\pi s (\Psi_{\lambda \mathbf{p}s}, \Psi_{\lambda \mathbf{p}'s'})_{KG} \quad (\text{A14})$$

and we may set $\lambda = 0$ to obtain an inner product on solutions to the Klein-Gordon equation. The Klein-Gordon inner product is of course positive on positive frequency ($s = 1$) solutions and negative on negative frequency ($s = -1$) solutions, but the form of the above result, with the overall factor of s , ensures that the induced inner product is always positive.

Note that some caution is required in relation to Eqs.(A7) and (A10), since Eq.(A7) implies that

$$\begin{aligned} \langle \lambda \mathbf{p}s | (\hat{p}^0 \delta(\hat{x}^0) + \delta(\hat{x}^0) \hat{p}^0) | \lambda' \mathbf{p}'s' \rangle &= i \langle \lambda \mathbf{p}s | [H, \theta(\hat{x}^0)] | \lambda' \mathbf{p}'s' \rangle \\ &= i(\lambda - \lambda') \langle \lambda \mathbf{p}s | \theta(\hat{x}^0) | \lambda' \mathbf{p}'s' \rangle \end{aligned} \quad (\text{A15})$$

This appears to be zero when $\lambda = \lambda'$ suggesting that Eq.(A10) is zero. This is not in fact the case since the inner product expression on the right-hand side of Eq.(A15) is actually divergent as $\lambda \rightarrow \lambda'$.

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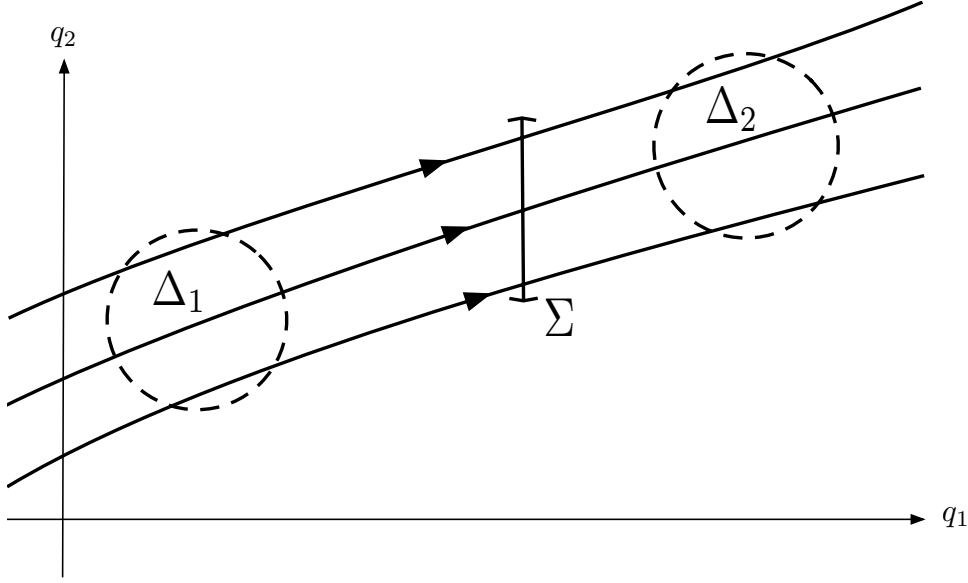


Figure 1. Given a solution Ψ to the Wheeler-DeWitt equation, what is the probability that the system enters a series of regions $\Delta_1, \Delta_2 \dots$ in configuration space, or crosses a surface Σ , at any stage in the system's entire history?

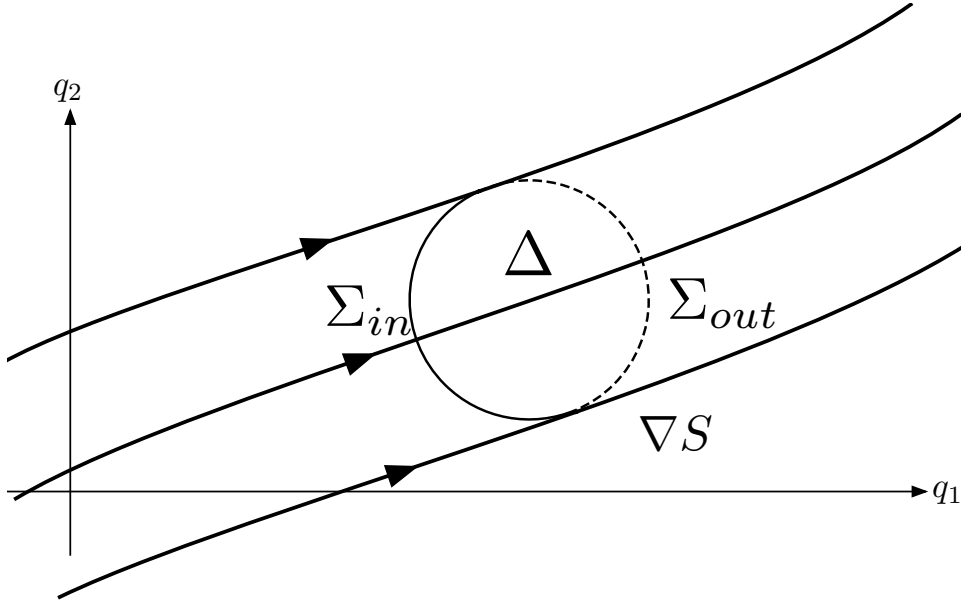


Figure 2. A WKB wave function with phase S corresponds to a set of classical trajectories with tangent vector ∇S . The probability for entering a region Δ is the amount flux of the wave function intersecting Δ . It may be expressed either in terms of the ingoing flux across Σ_{in} or equally, in terms of the outgoing flux across Σ_{out} .

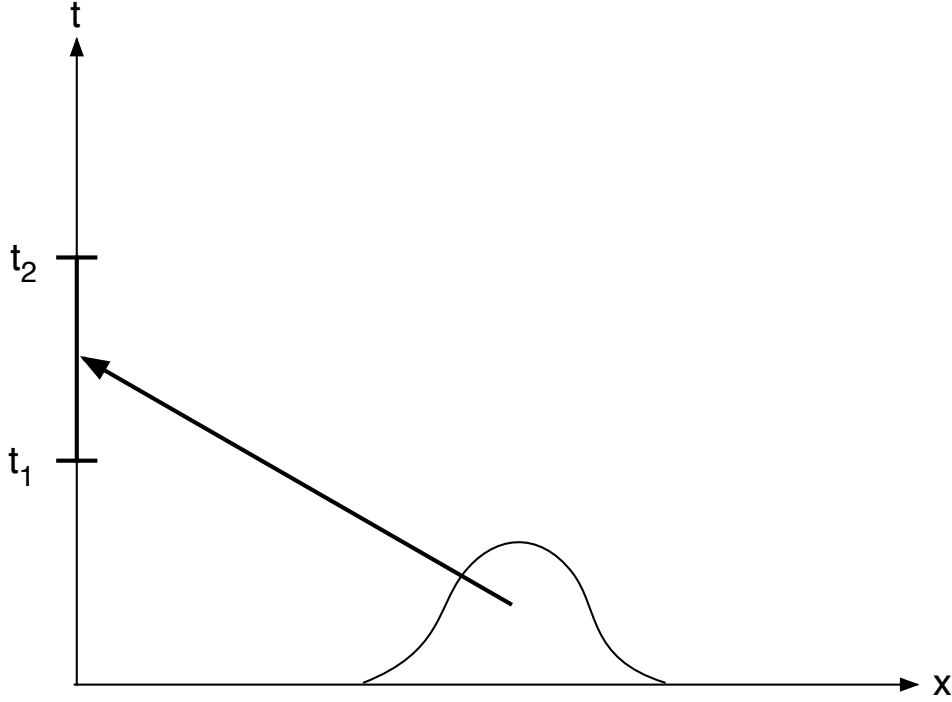


Figure 3. The quantum arrival time problem in non-relativistic quantum mechanics. Given an initial state localized entirely in $x > 0$ and consisting entirely of negative momenta, what is the probability that the particle crosses the origin during the time interval $[t_1, t_2]$?

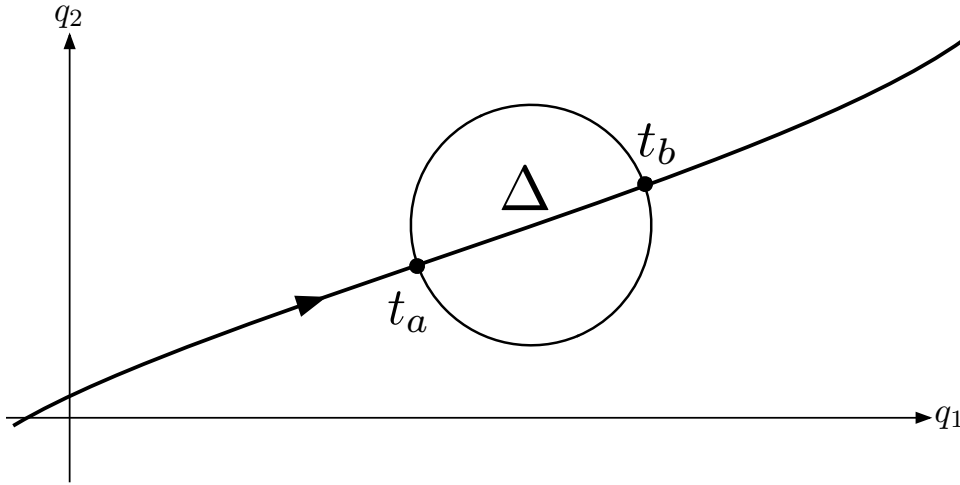


Figure 4. A classical trajectory $q^a(t)$ intersecting Δ enters at parameter time t_a and leaves at parameter time t_b .

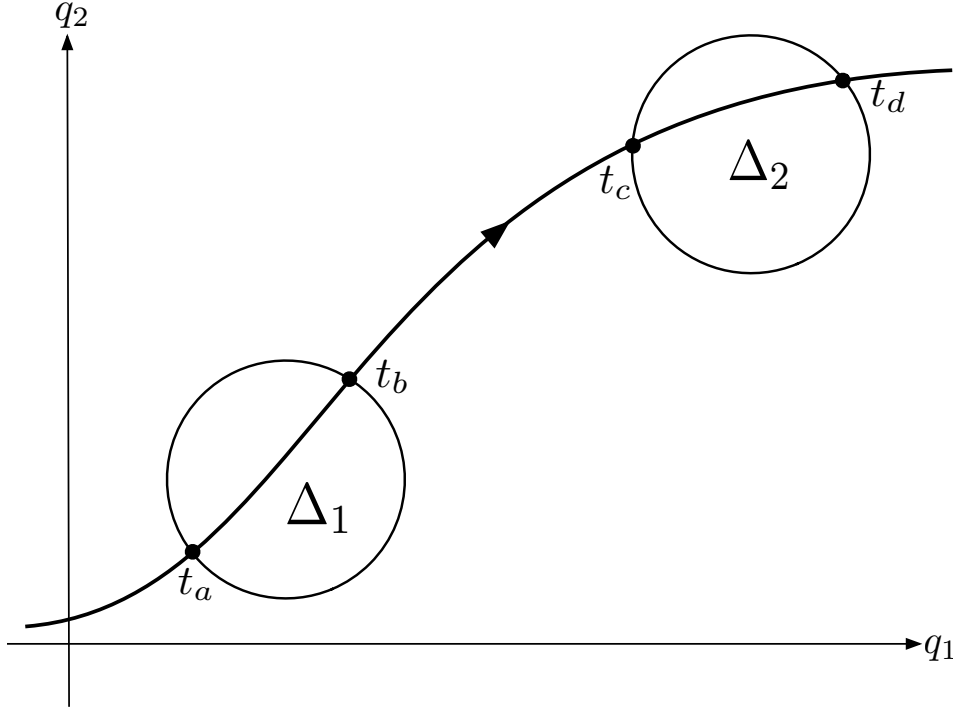


Figure 5. A classical trajectory $q^a(t)$ intersecting Δ_1 and Δ_2 enters Δ_1 at t_a , leaves at t_b , enters Δ_2 at t_c and leaves at t_d .

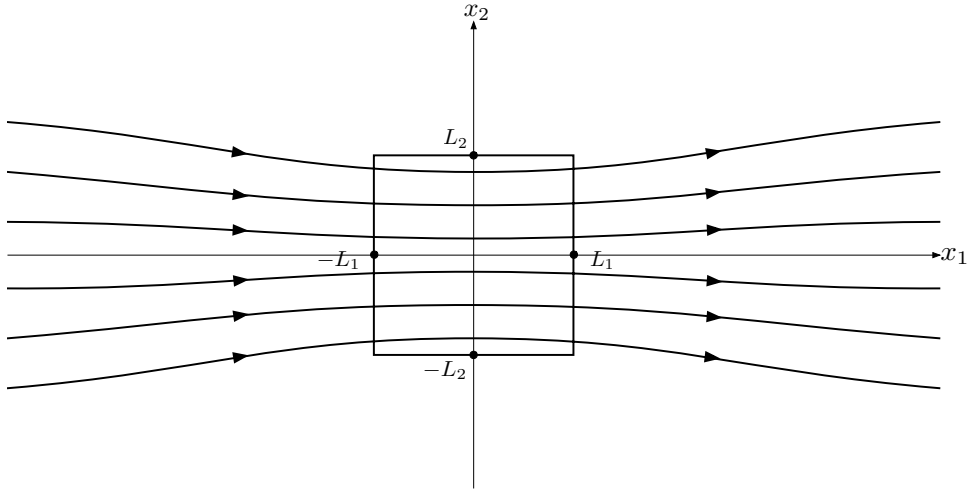


Figure 6. The class operator C_Δ acting on the initial state $|\Psi\rangle$ produces a state consisting of a plane wave $\exp(ip_1 x_1)$ localized along a tube of width $2L_2$ centred around the x_1 axis, with spreading through a small angle as $x_1 \rightarrow \pm\infty$.

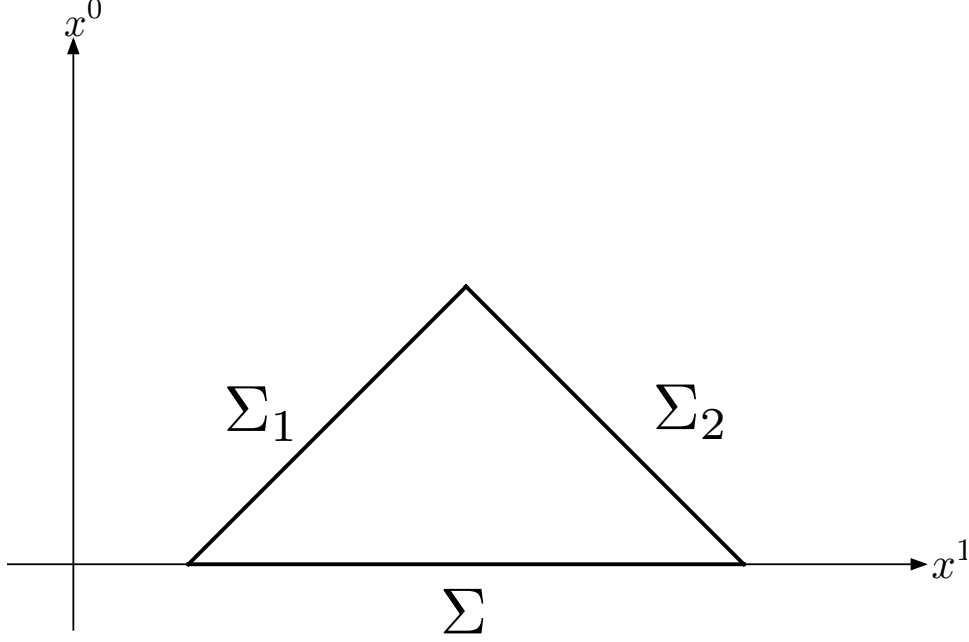


Figure 7. The class operator for a relativistic particle to cross a surface Σ may be calculated by regarding Σ as part of the boundary of the spacetime region Δ , a section of null cone whose base is Σ . In two dimensions, depicted here, it is a triangle with base Σ whose other two sides are the null surfaces Σ_1, Σ_2 .

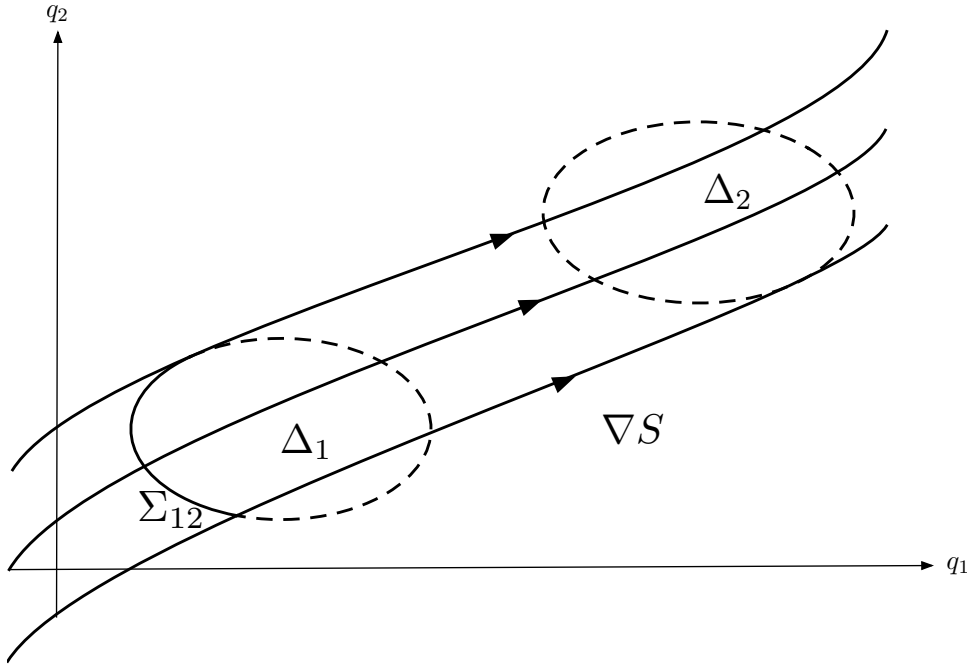


Figure 8. The class operator $C_{\Delta_1 \Delta_2}$ for two regions operating on a WKB wave function produces another WKB state localized around the flux passing through both regions. This is the same as the flux entering Δ_1 across the surface Σ_{12} .